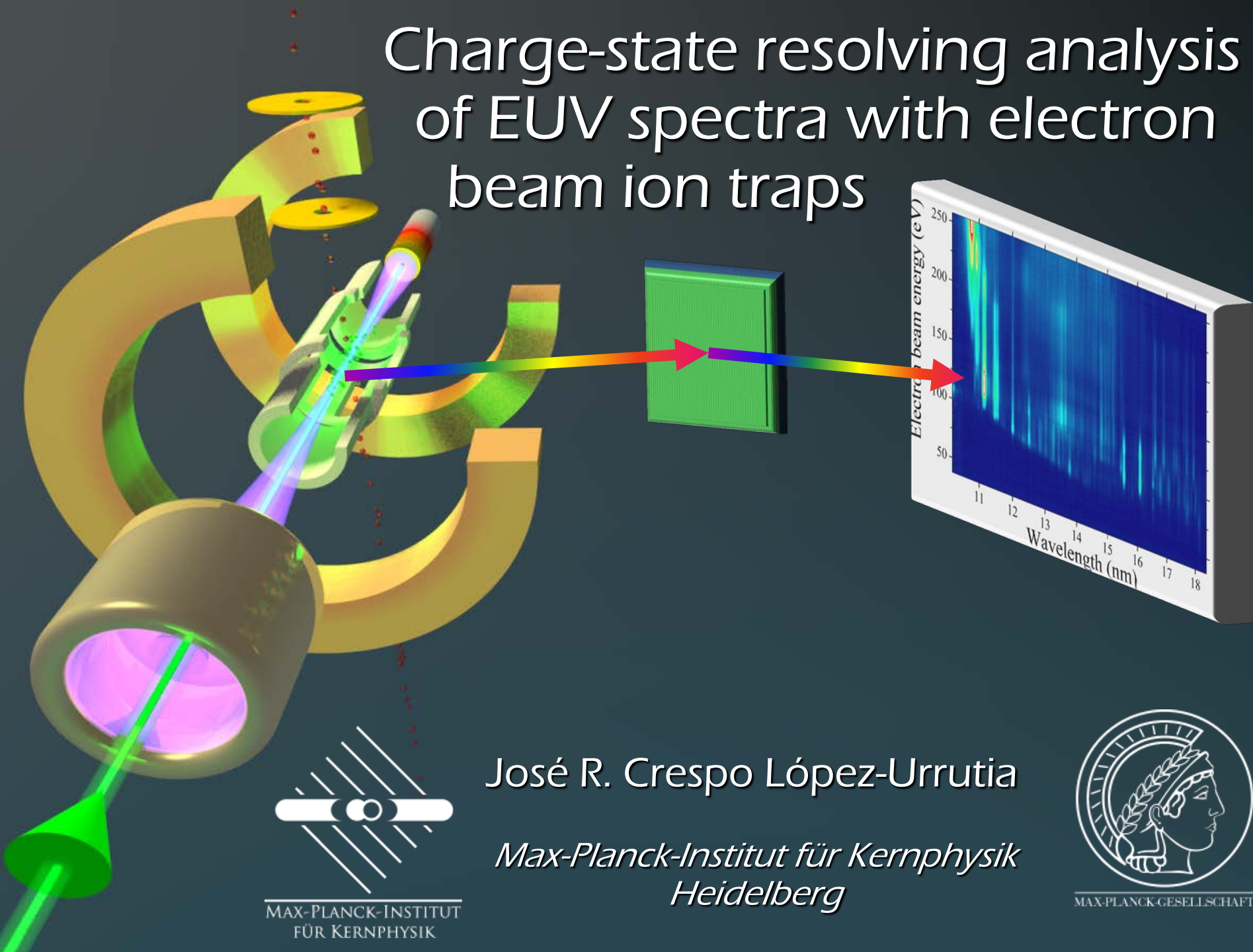


# Charge-state resolving analysis of EUV spectra with electron beam ion traps



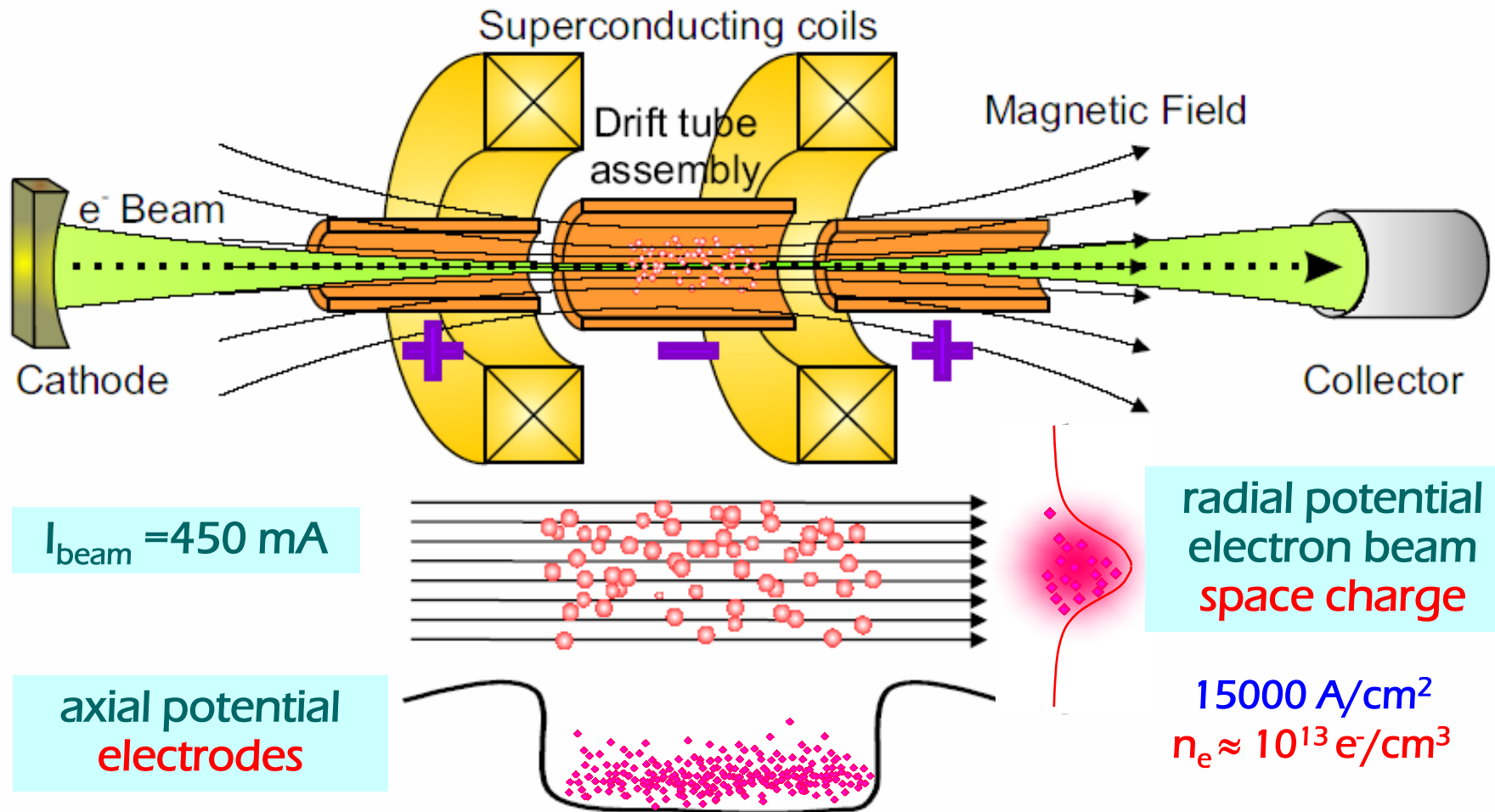
José R. Crespo López-Urrutia

*Max-Planck-Institut für Kernphysik  
Heidelberg*

# Overview

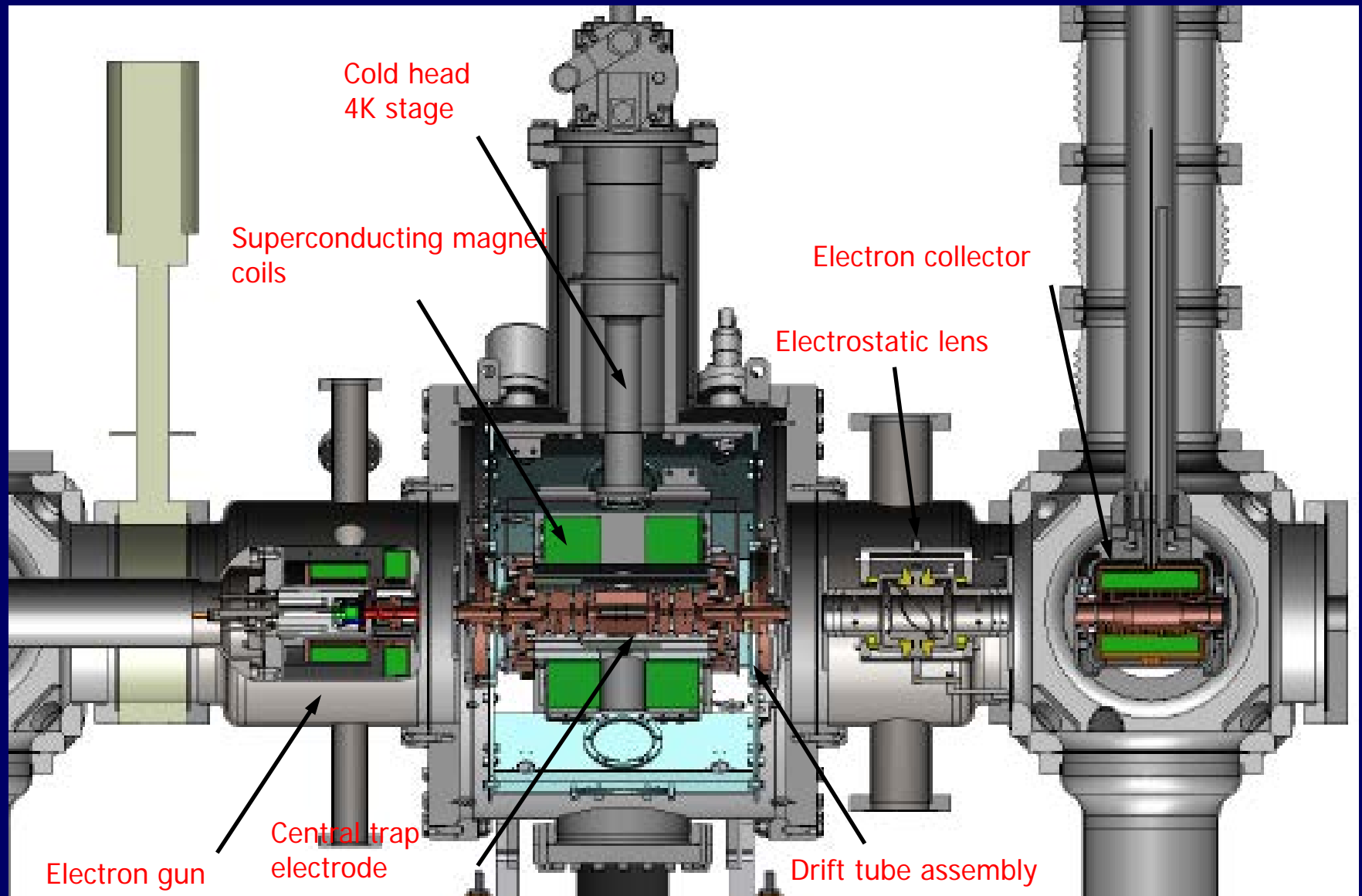
- Electron beam ion traps
- Photon excitation studies
- Electron excitation studies
- Optical and EUV spectroscopy of Sn
- Conclusions

# HCl production with electron beam ion trap



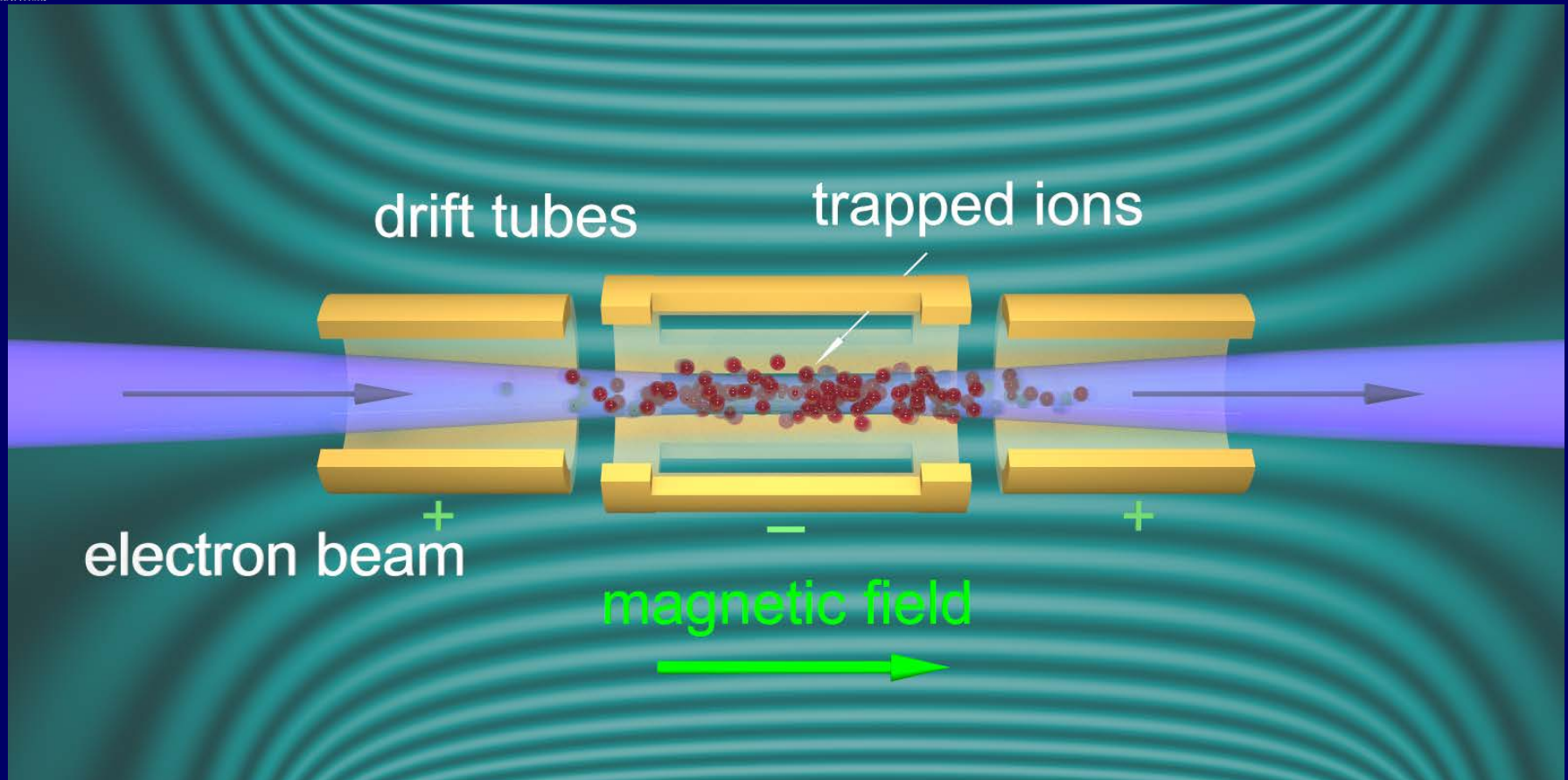
Electron beam drives ionization, excites and traps the ions inside a cylindrical volume

# EBIT design MPIK Heidelberg



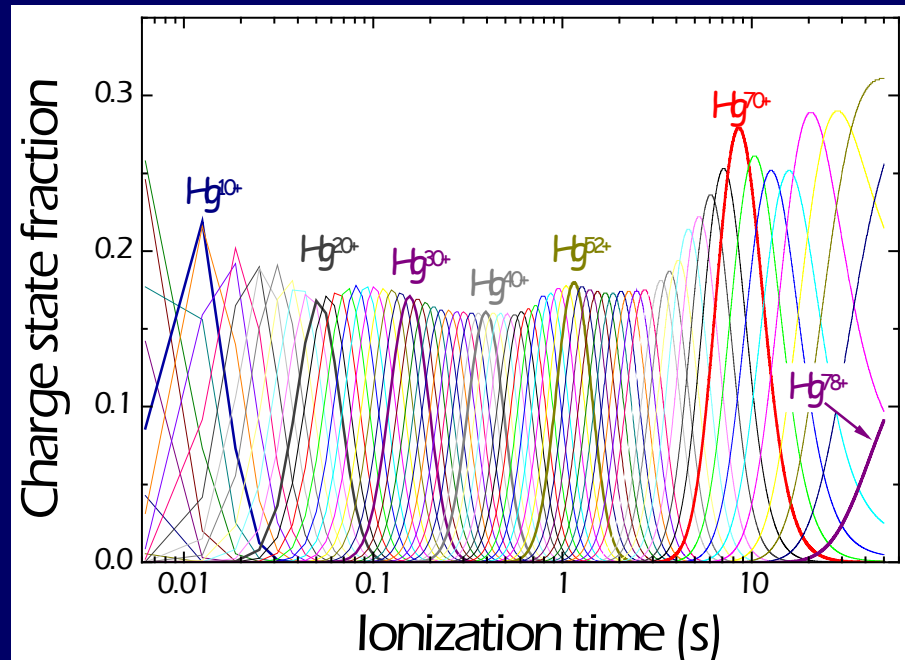


# HCl production with electron beam ion trap



Electron beam drives ionization, excites and traps the ions inside a cylindrical volume

# Time evolution of the charge state

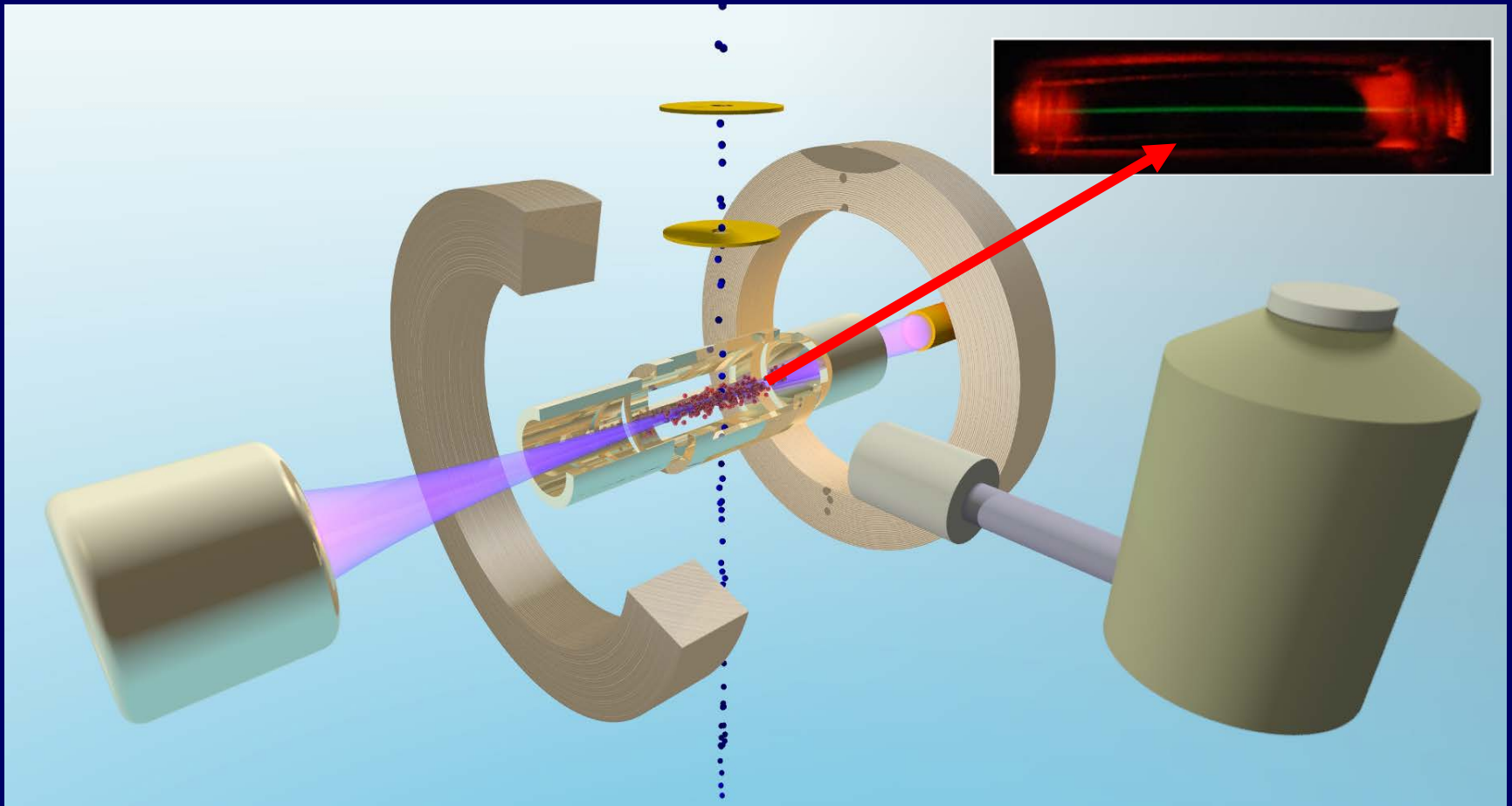


- Time evolution of mean charge state **governed by electron beam energy** (microsecond to second scale)
- Unscrambling atomic physics processes possible due to **monoenergetic electron beam** ( $E/\Delta E \approx 1000$ )

$$\frac{dn_0}{dt} = -n_0\sigma_{0,1}j_e$$

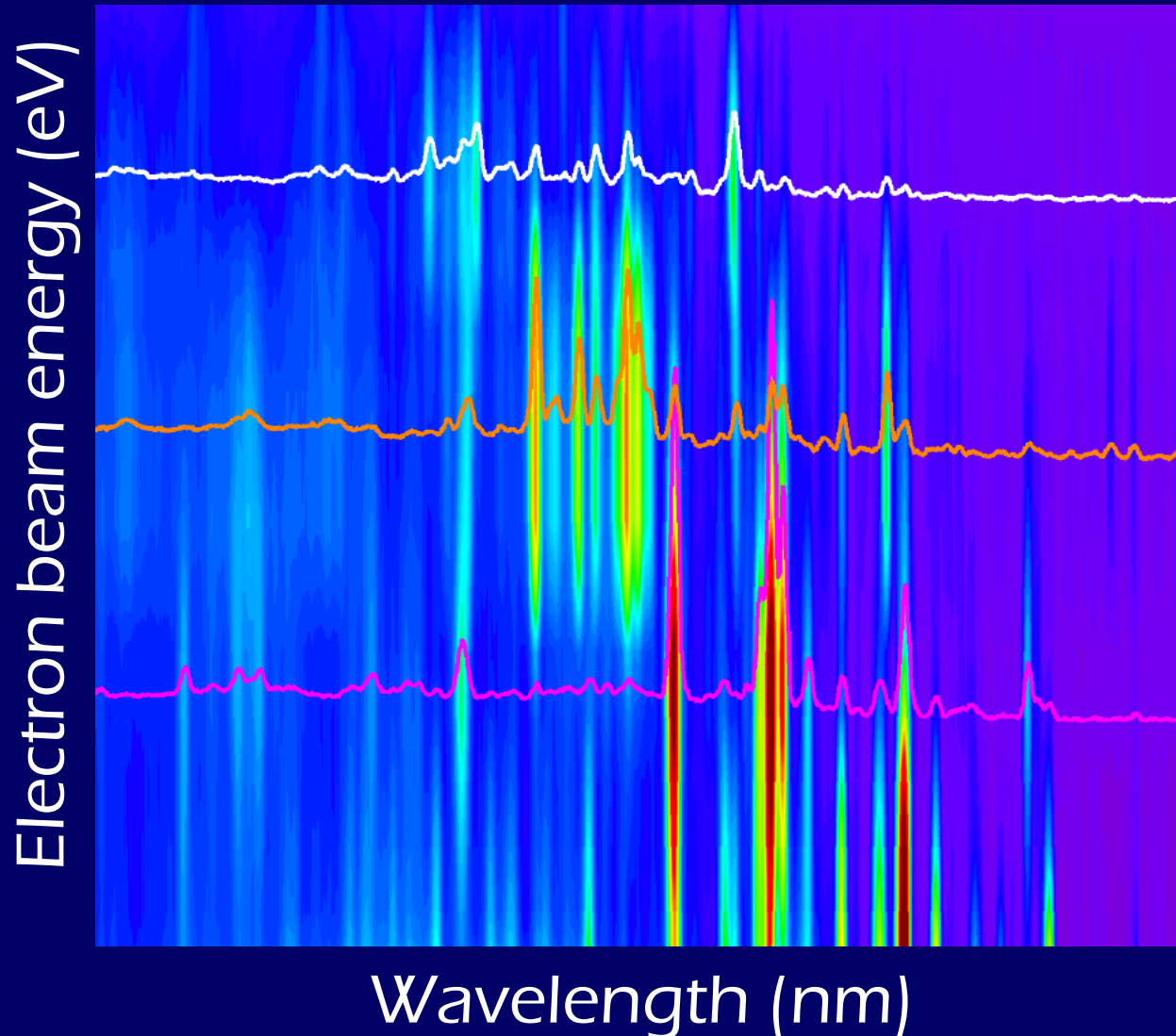
$$\frac{dn_Z}{dt} = n_{Z-1}\sigma_{Z-1,Z}j_e - n_Z\sigma_{Z,Z+1}j_e - \frac{n_Z}{\tau_{rec}(q)}$$

# Strong excitation by electron impact and resonant photorecombination



Ge, Si detectors, crystal and grating spectrometers, microcalorimeters, etc., for X-ray diagnostics

# Choice of charge state by dialing electron beam energy



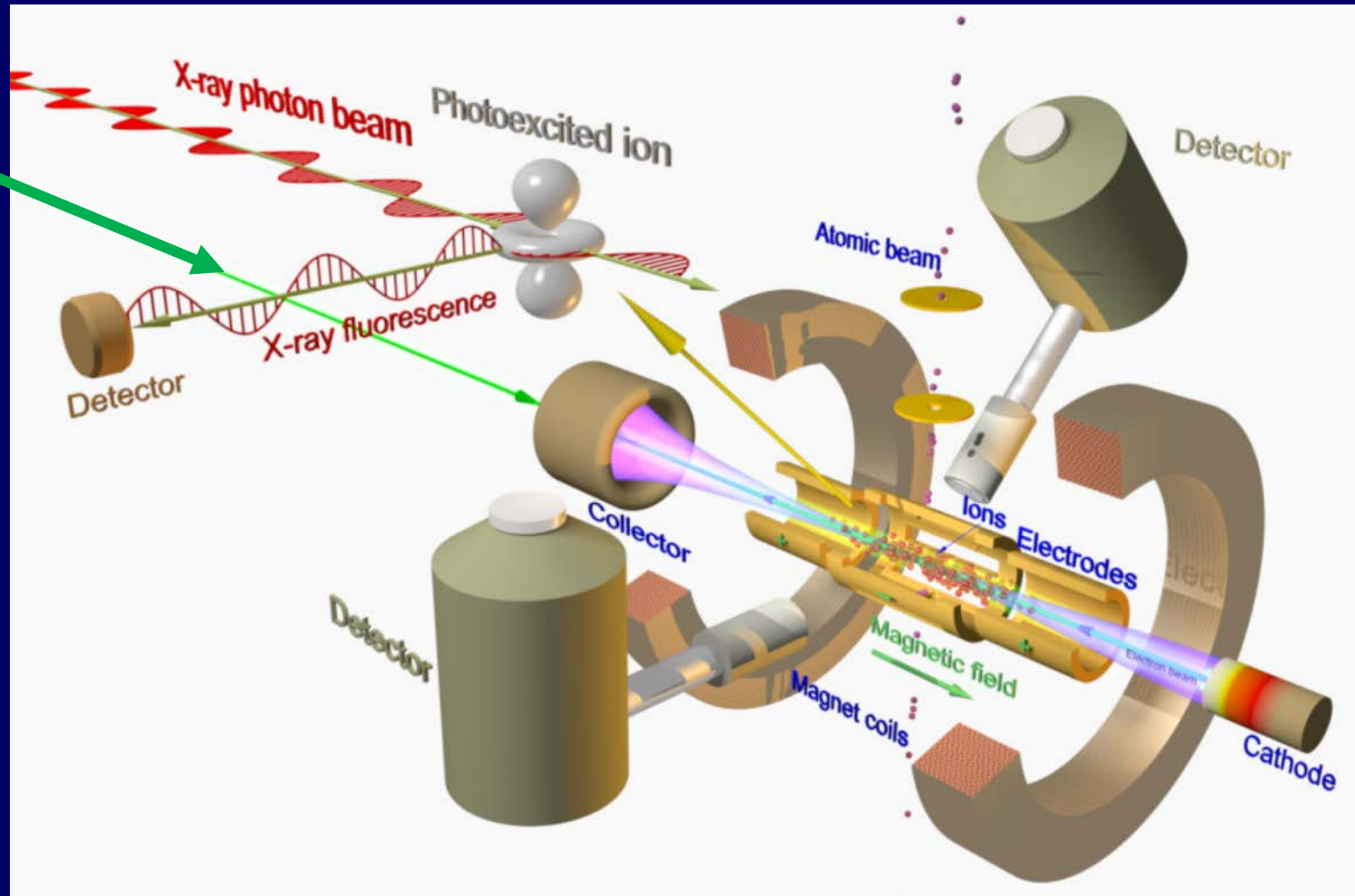
# What we do with EBITs

- Photorecombination processes: **radiative + dielectronic, trielectronic and quadruelectronic recombination**,
- **Photoionization of HCl** with synchrotron radiation, from  $N^{3+}$  (from 60 eV) to  $Kr^{33+}$  (at 14 keV)
- High-resolution spectroscopy **from optical to X-rays**
- **Free-electron laser soft x-ray spectroscopy** (<800 eV)
- High-resolution x-ray metrology with synchrotron radiation (<14.4 keV)
- **Laser spectroscopy** of forbidden optical lines in HCl
- **Sympathetic cooling of HCl** for frequency metrology
- **Charge-exchange** studies

# Free-electron laser and synchrotron-radiation excitation and photoionization of highly charged ions



# Resonant **photon excitation** in EBIT



- Synchrotron radiation (PETRAIII),
  - Free-electron lasers (LCLS) ,
- provide **X-rays with high power and energy resolution**

# Photon diagnostics

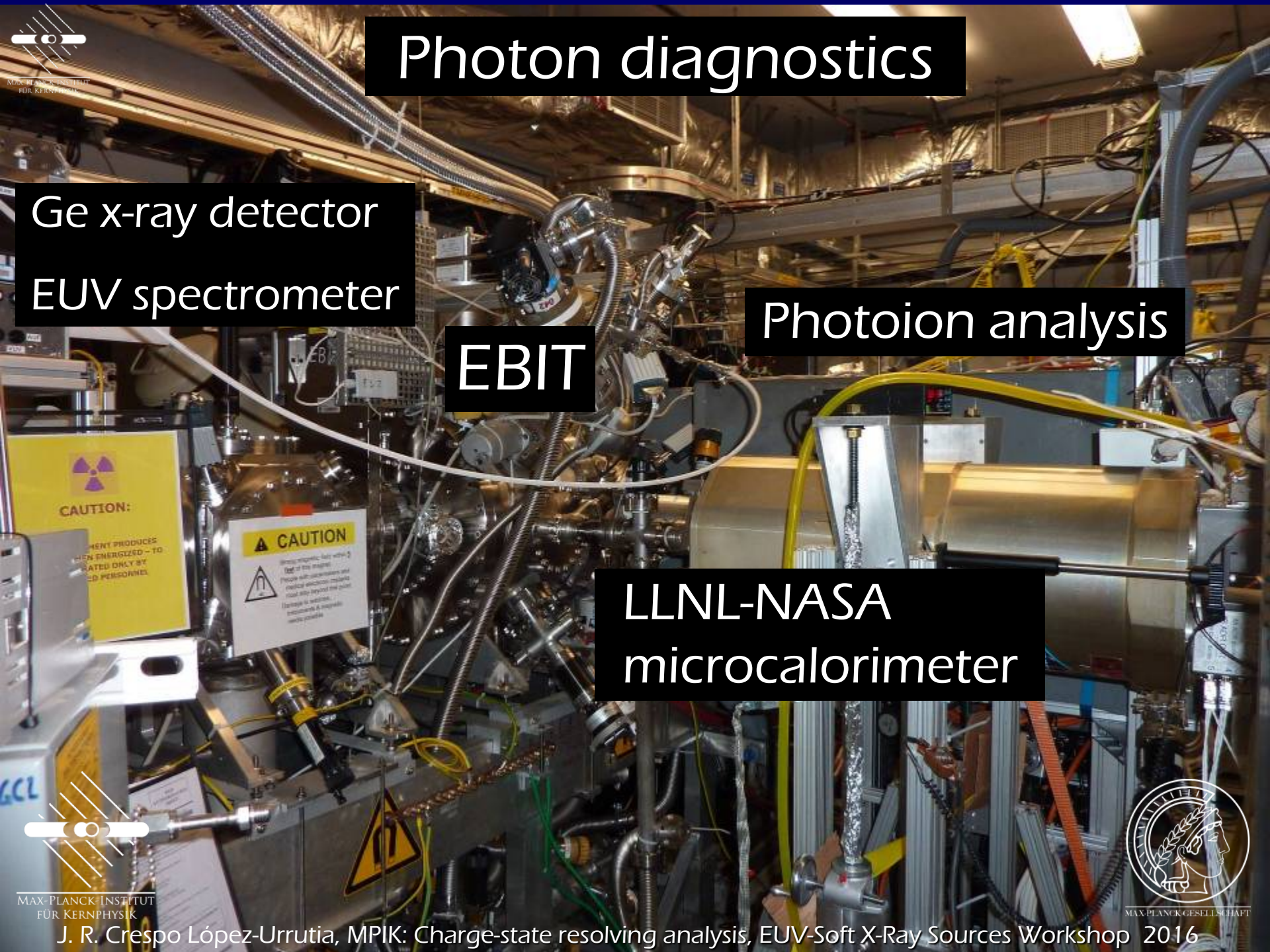
Ge x-ray detector

EUV spectrometer

EBIT

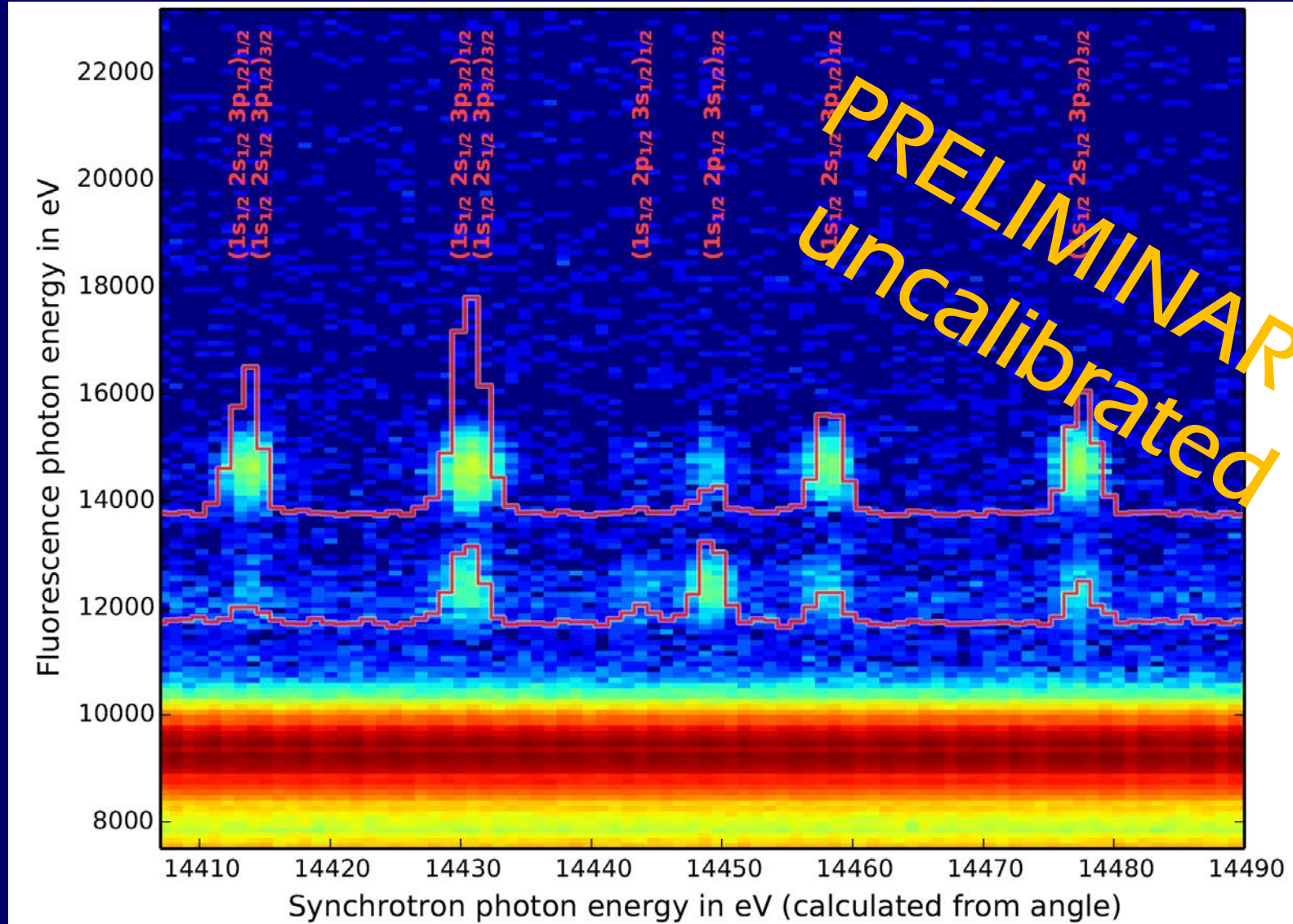
Photoion analysis

LLNL-NASA  
microcalorimeter





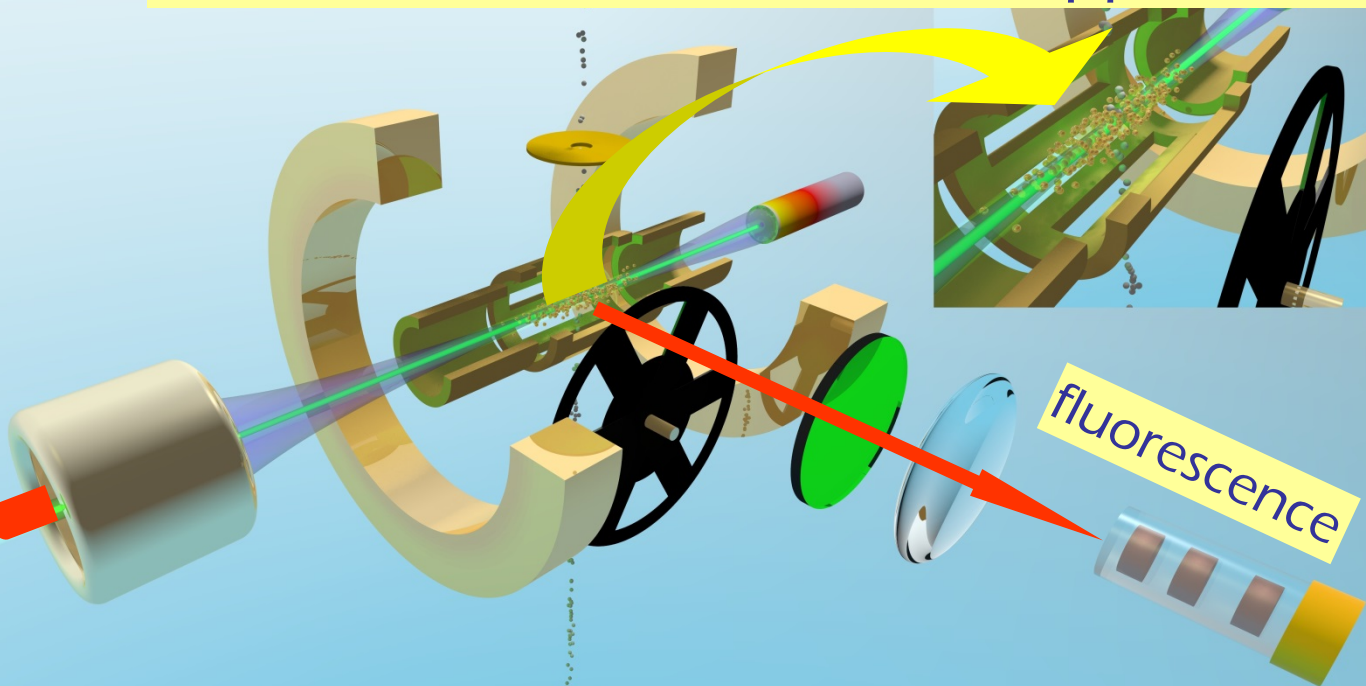
# New results: Overview spectra of $\text{Br}^{33+}$ (Li-like)



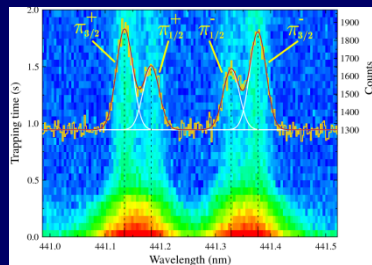
S. Bernitt, MPIK (2016)

photoions

LCLS,  
BESSY II,  
Petra III,  
lasers

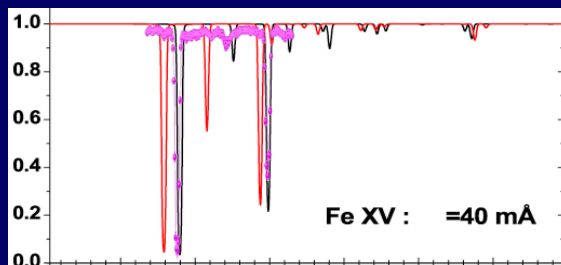


Visible M1  
Ar<sup>13+</sup>



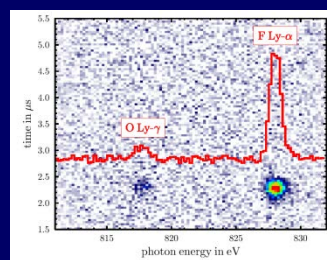
V. Mäkel et al.,  
PRL **107** 143002  
(2011)

# Soft X-ray photoionization



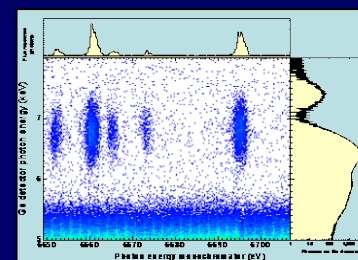
M. C. Simon et al.,  
PRL 105 183001  
(2010)

FEL 800 eV  
Fe<sup>16+</sup>



S. Bernitt et al.,  
Nature **492**, 225  
(2012)

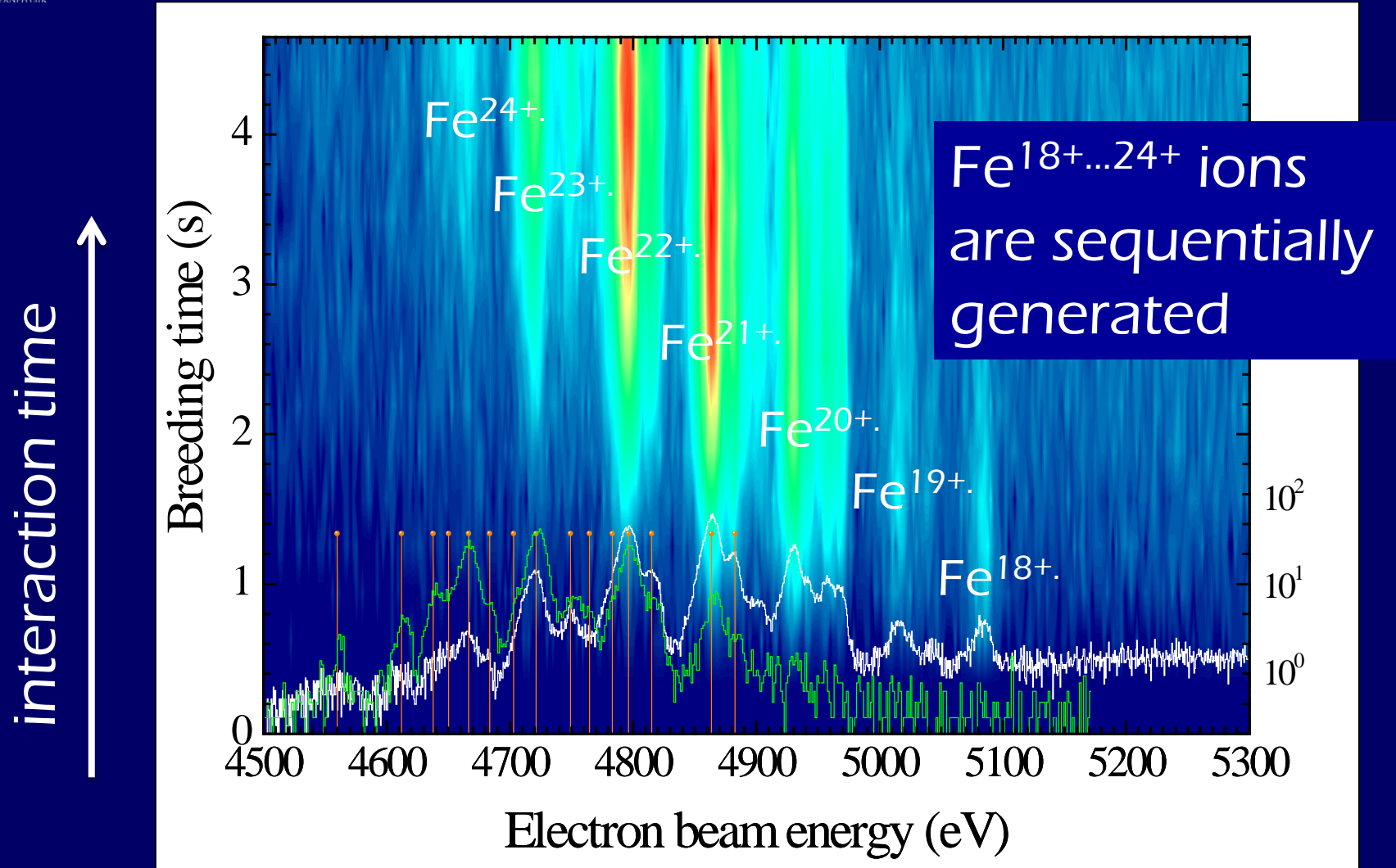
Synchrotron 6 keV  
Fe<sup>24+</sup>, 13 keV Kr<sup>34+</sup>



J. Rudolph et al.,  
PRL 111, 103002  
(2013)

# Electron-driven resonant processes

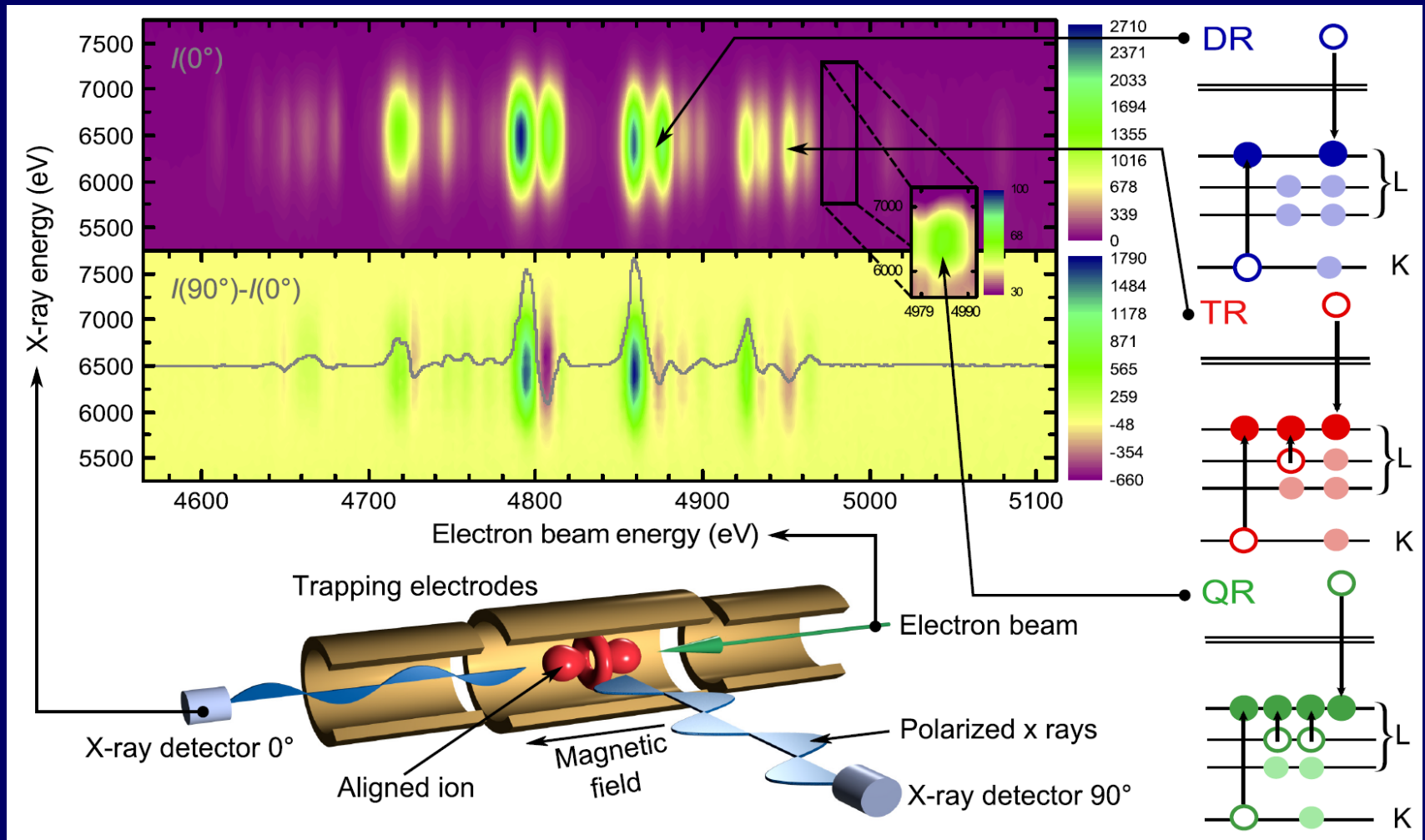
# X-ray data depending on electron energy



Ions in any desired charge state can be prepared, stored and spectroscopically studied

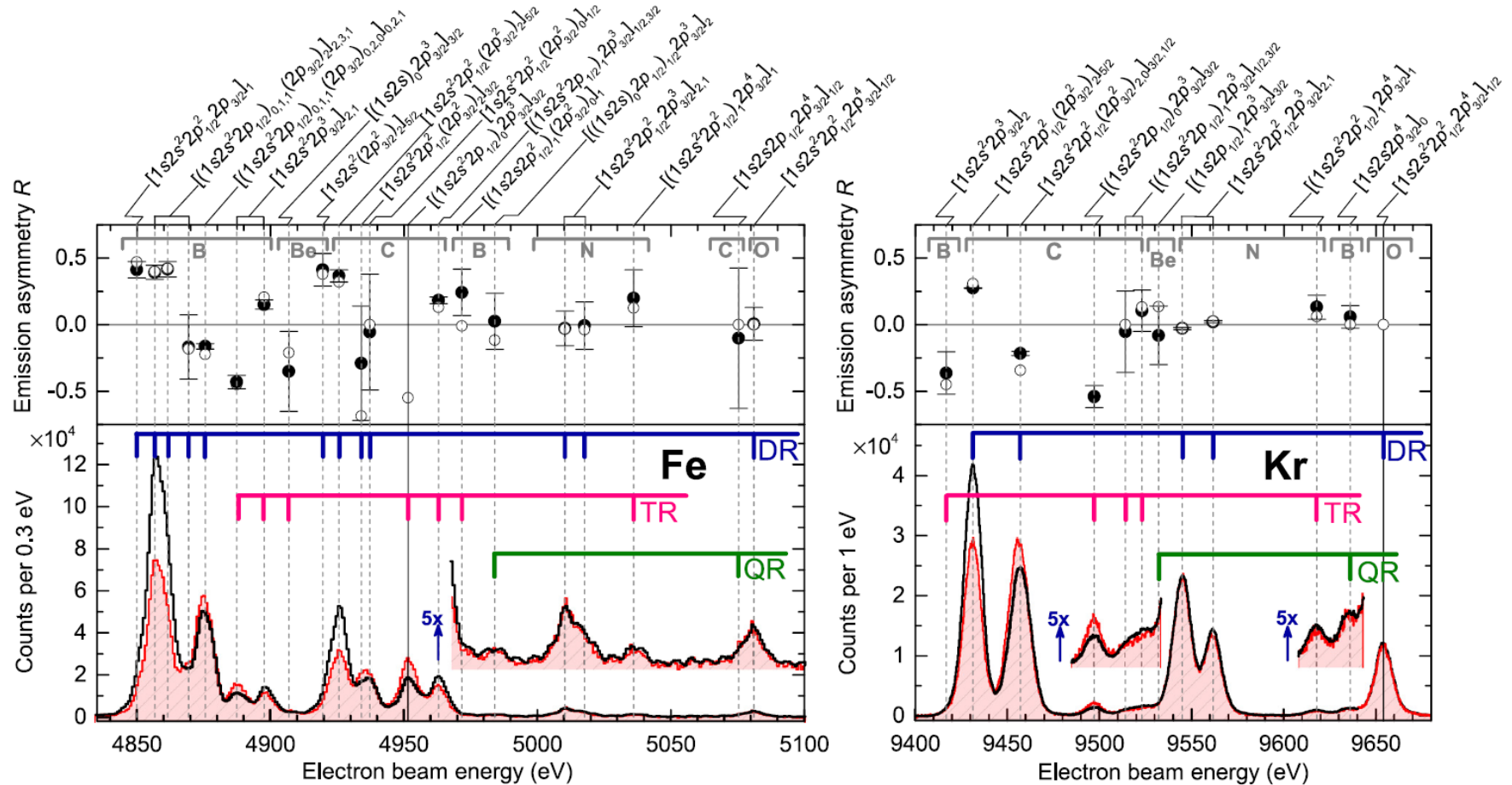


# Unexpected, strong contributions by many-electron resonant excitation at high resolution



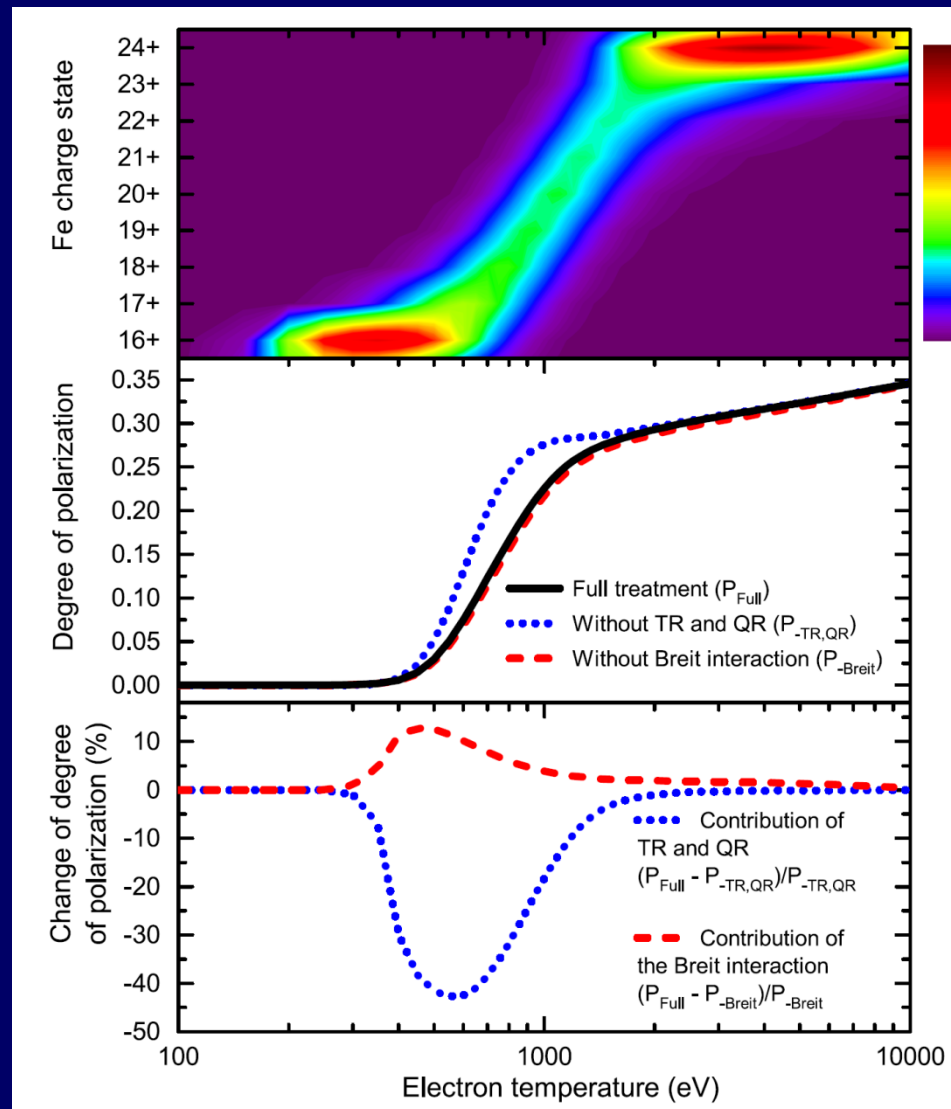
C. Shah et al., Phys. Rev. E **93**, 061201(R) (2016)  
 C. Beilmann et al., Phys. Rev. Lett **107**, 143201 (2011)  
 C. Beilmann et al., Phys. Rev. A **88**, 062706 (2013)

Unexpected, strong contributions by  
many-electron resonant excitation at high resolution



C. Shah et al., Phys. Rev. E **93**, 061201(R) (2016)  
C. Beilmann et al., Phys. Rev. Lett **107**, 143201 (2011)  
C. Beilmann et al., Phys. Rev. A **88**, 062706 (2013)

# Mean charge state of plasmas changed by many-electron resonant excitation



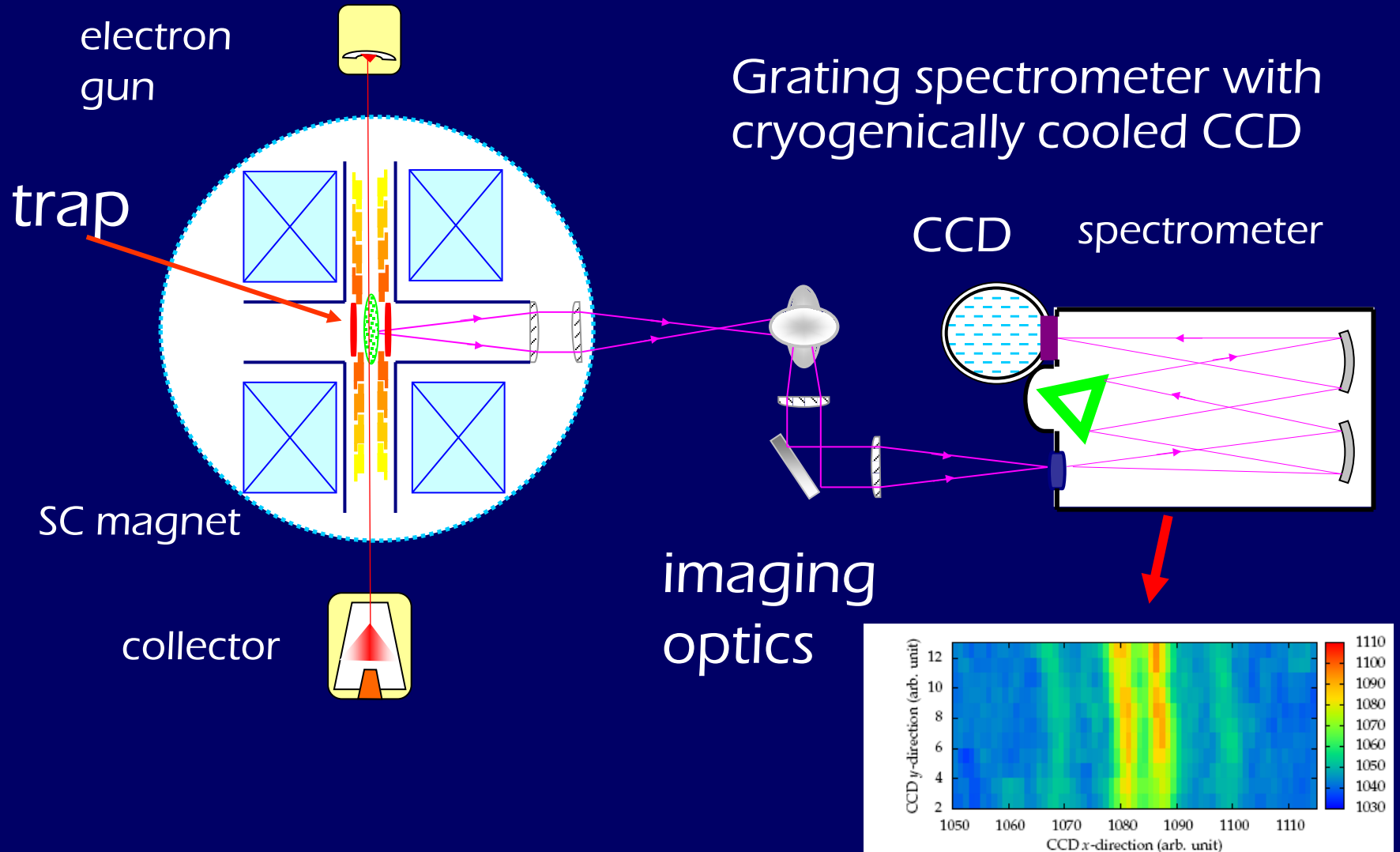
C. Shah et al.,  
Phys. Rev. E **93**,  
061201(R)  
(2016)

# Conclusions from FEL, synchrotron and photorecombination studies

- Previously known but neglected **complex multielectron processes have experimentally shown unexpectedly strong contributions** to both photorecombination and photoionization
- Inclusion of those channels in calculations is **necessary to achieve agreement** with existing experimental data
- Even the most advanced theoretical methods are **not as accurate as the experiments**
- Achieving agreement at the 1% (energies) respectively 5% (cross sections) levels will require **more dedicated theoretical work and benchmarking experimental data**

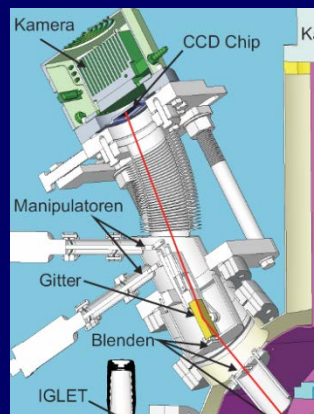
# Optical and EUV spectroscopy with EBITs

# Spectroscopy of few-electron ions in the visible range





# Electron beam ion trap diagnostics

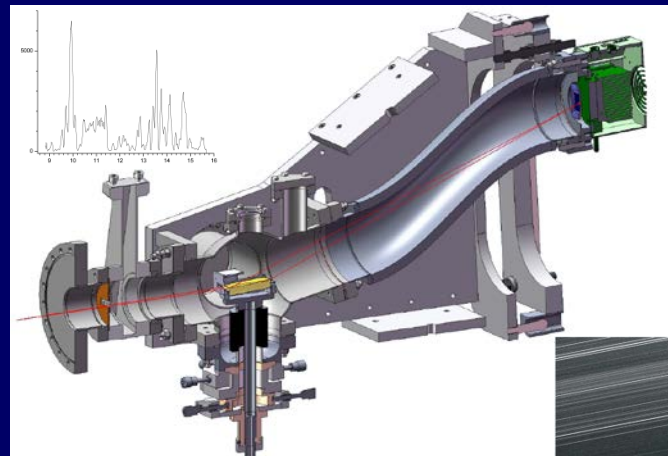


EUV grating spectrometer 1

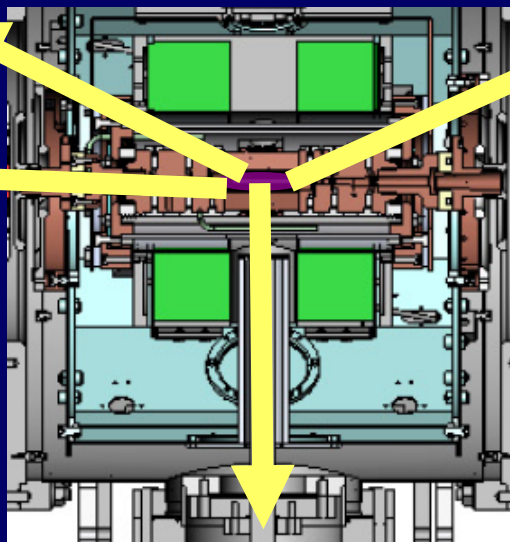
EUV to  
soft X-ray

EUV

EUV grating spectrometer 2



X-ray



X-ray

Silicon drift detector  
Germanium detector

Si drift detector, Ge detector

X-ray photons 1 to 30 keV

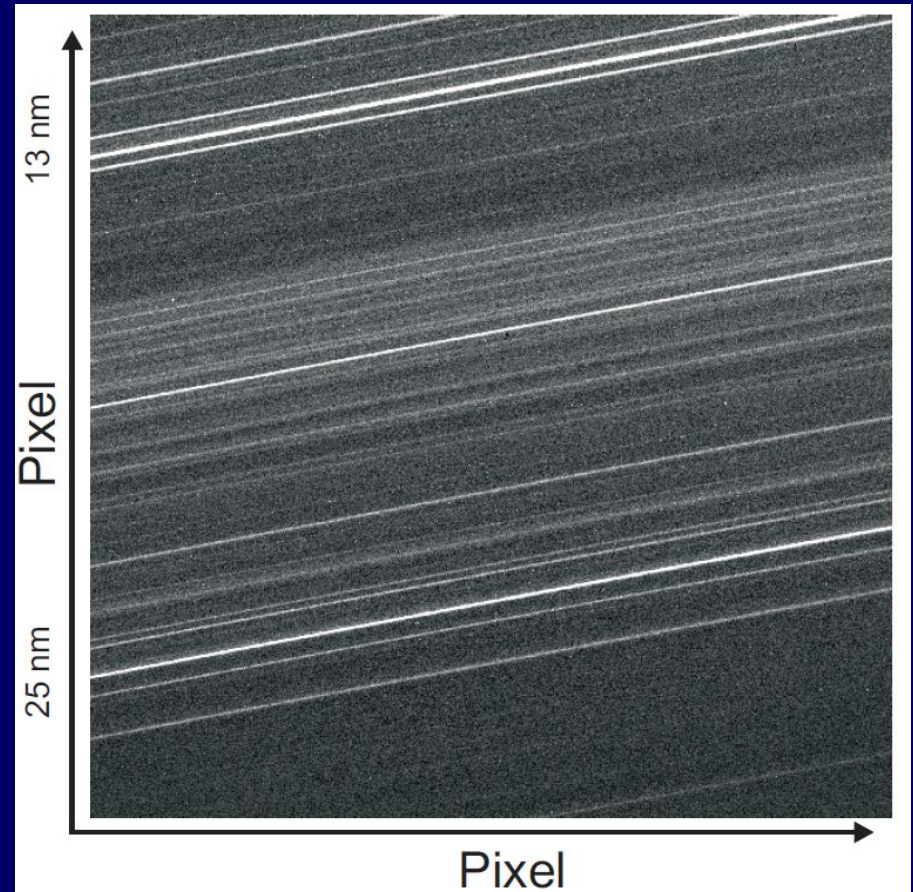
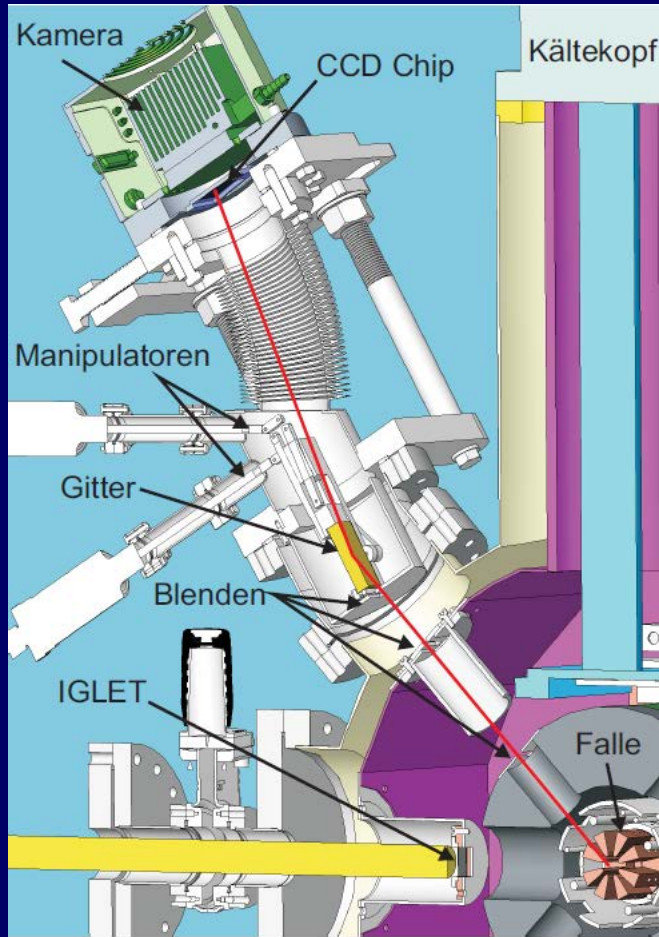
Two grating spectrometers

EUV photons 40 eV to 1 keV

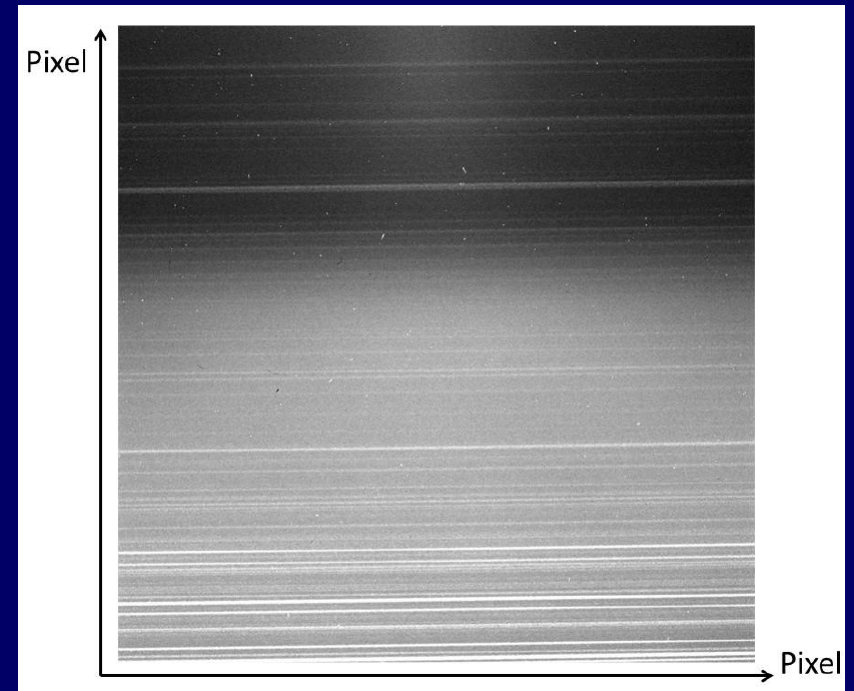
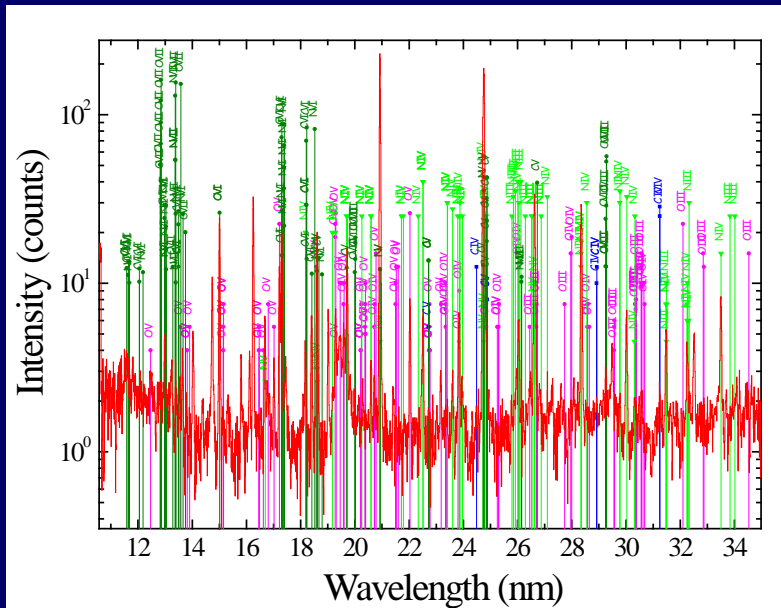
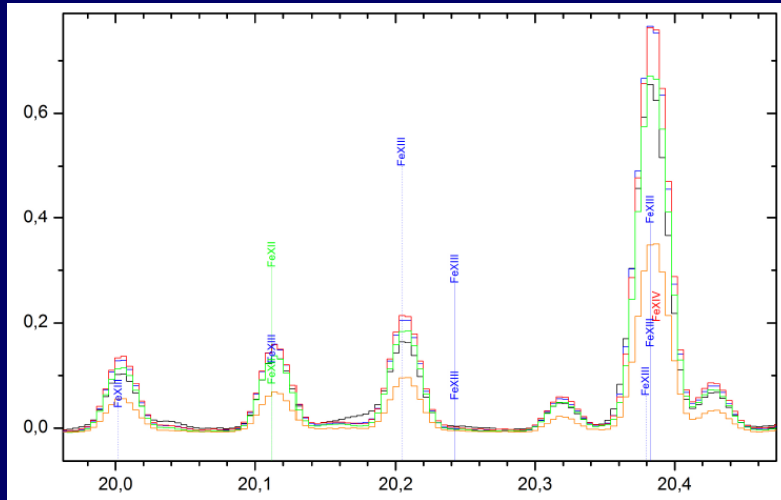
Metallic magnetic microcalorimeter

X-ray photons 2 to 8 keV

# EUV diagnostics



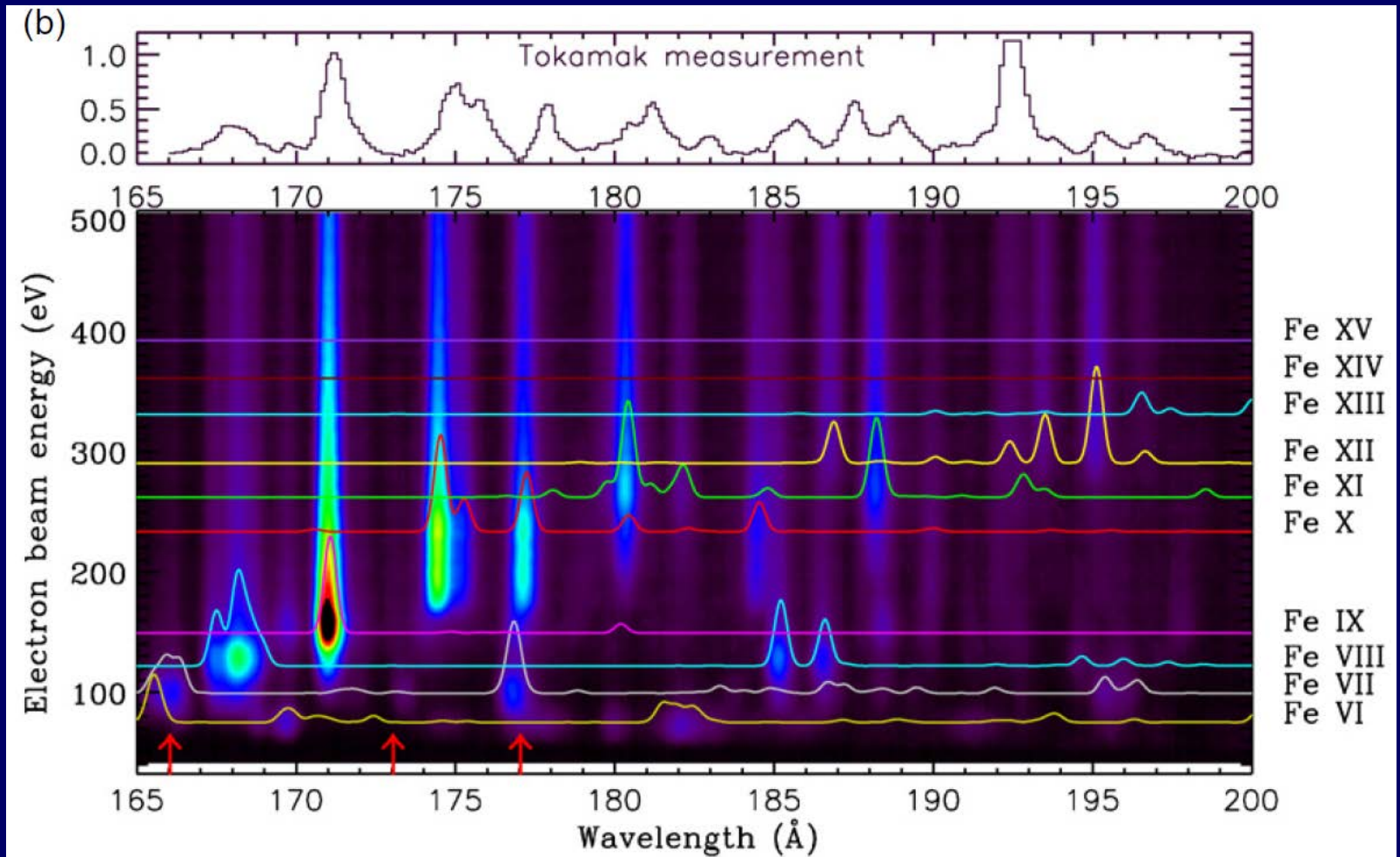
# EUV diagnostics



# Calibration lines of O and N

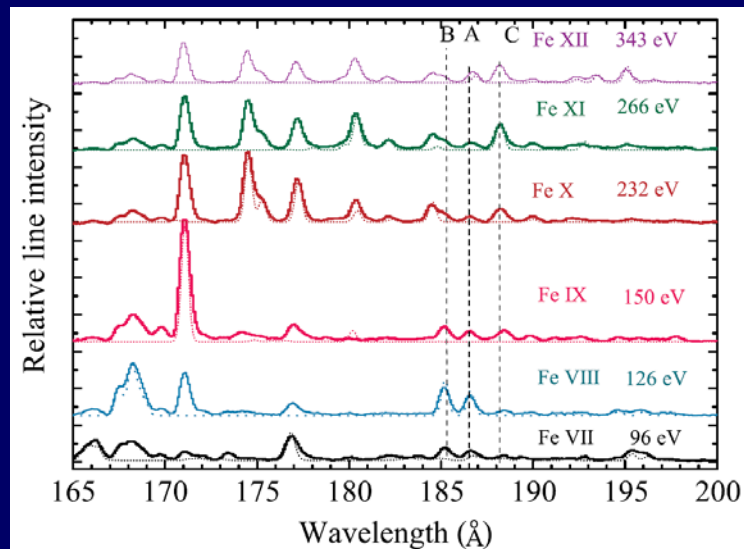
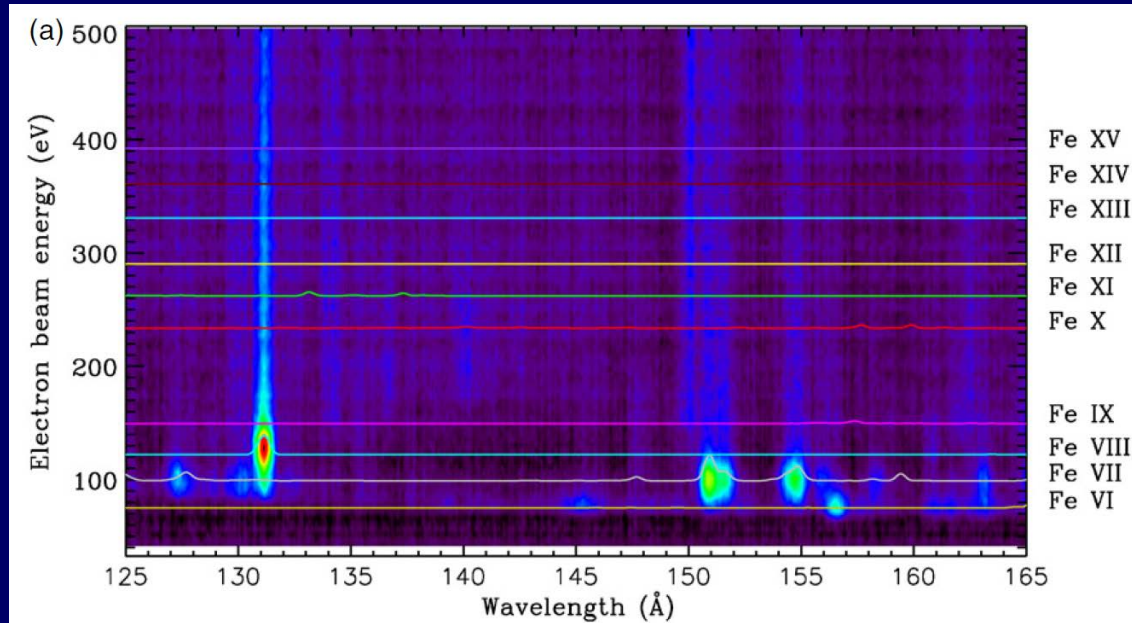


# Studies of Fe HCl with charge-state resolution



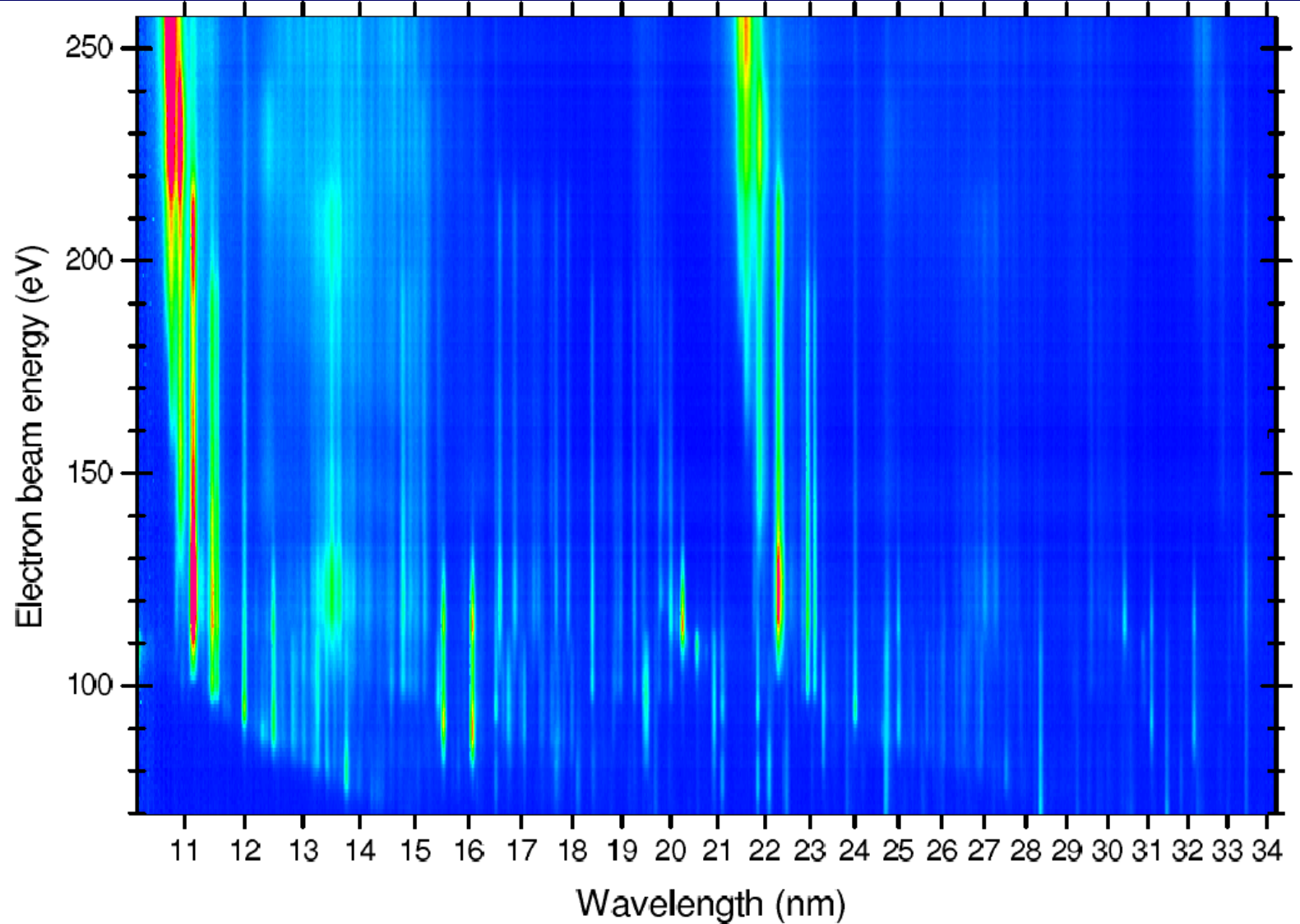
Gu et al., *Astrophys. J.* 696, 2275 (2009)

# Studies of Fe HCl with charge-state resolution



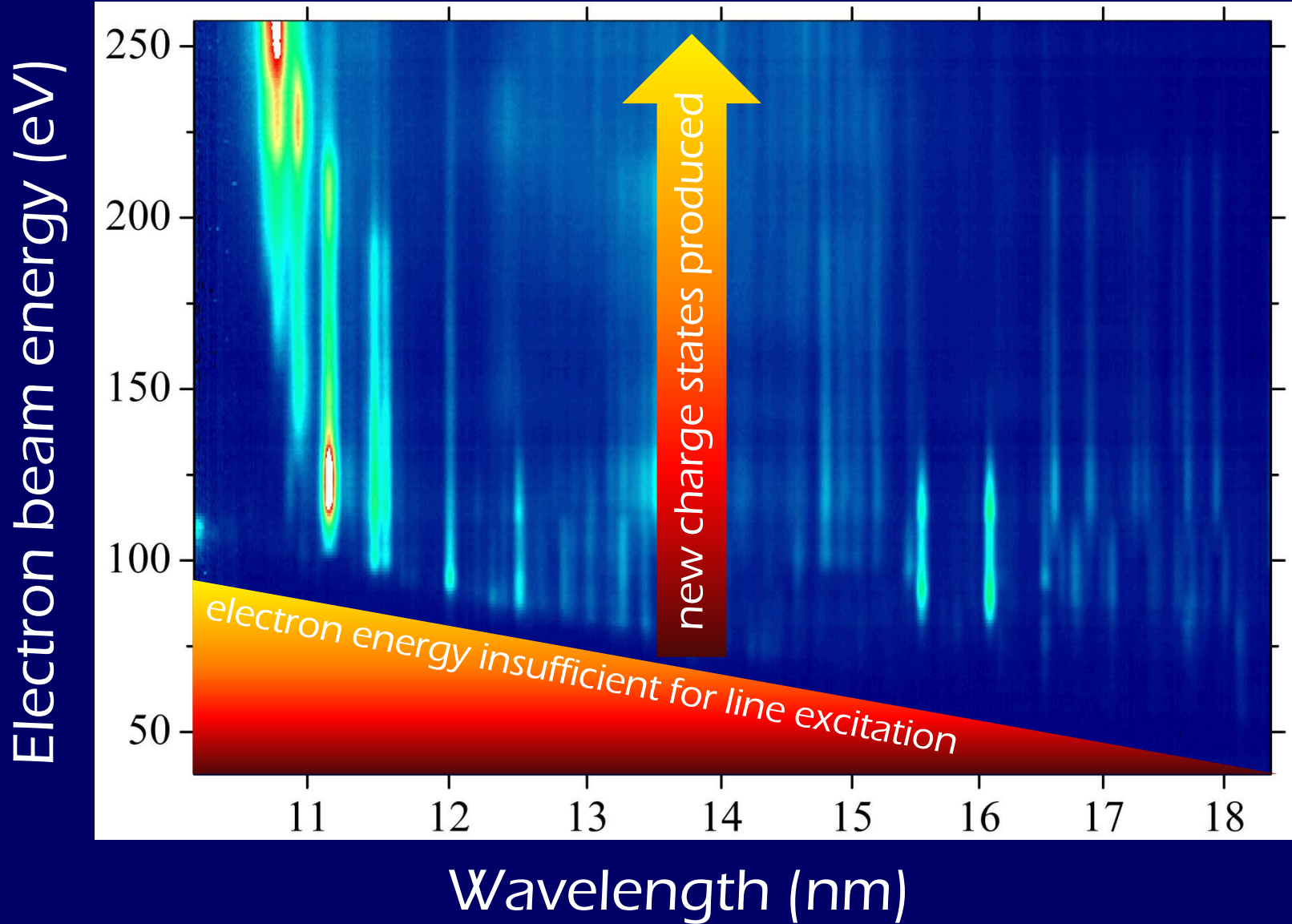
Gu et al., *Astrophys. J.* 696,  
2275 (2009)

# Charge state resolved spectra of Xe

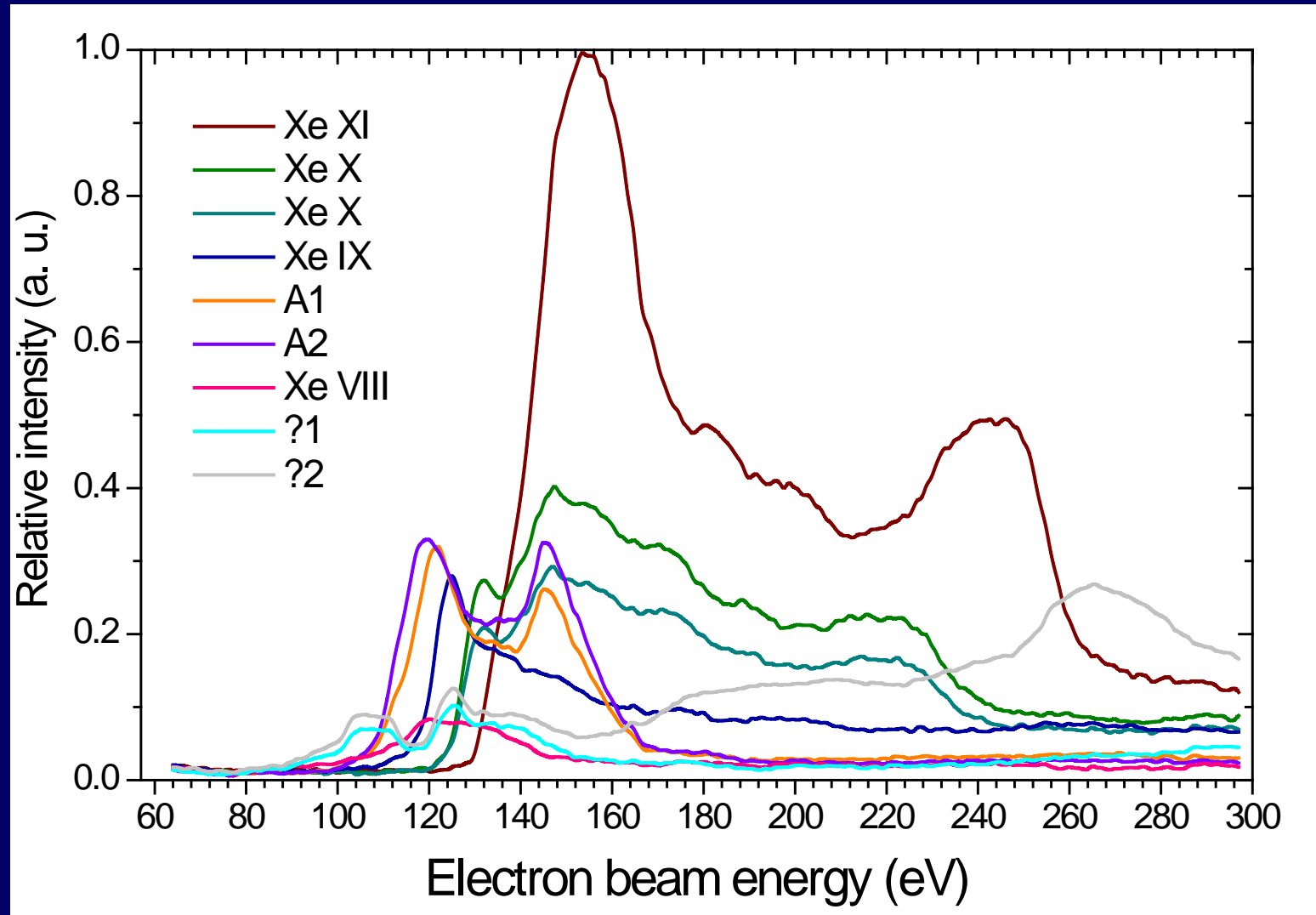




# Charge state resolved spectra of Xe

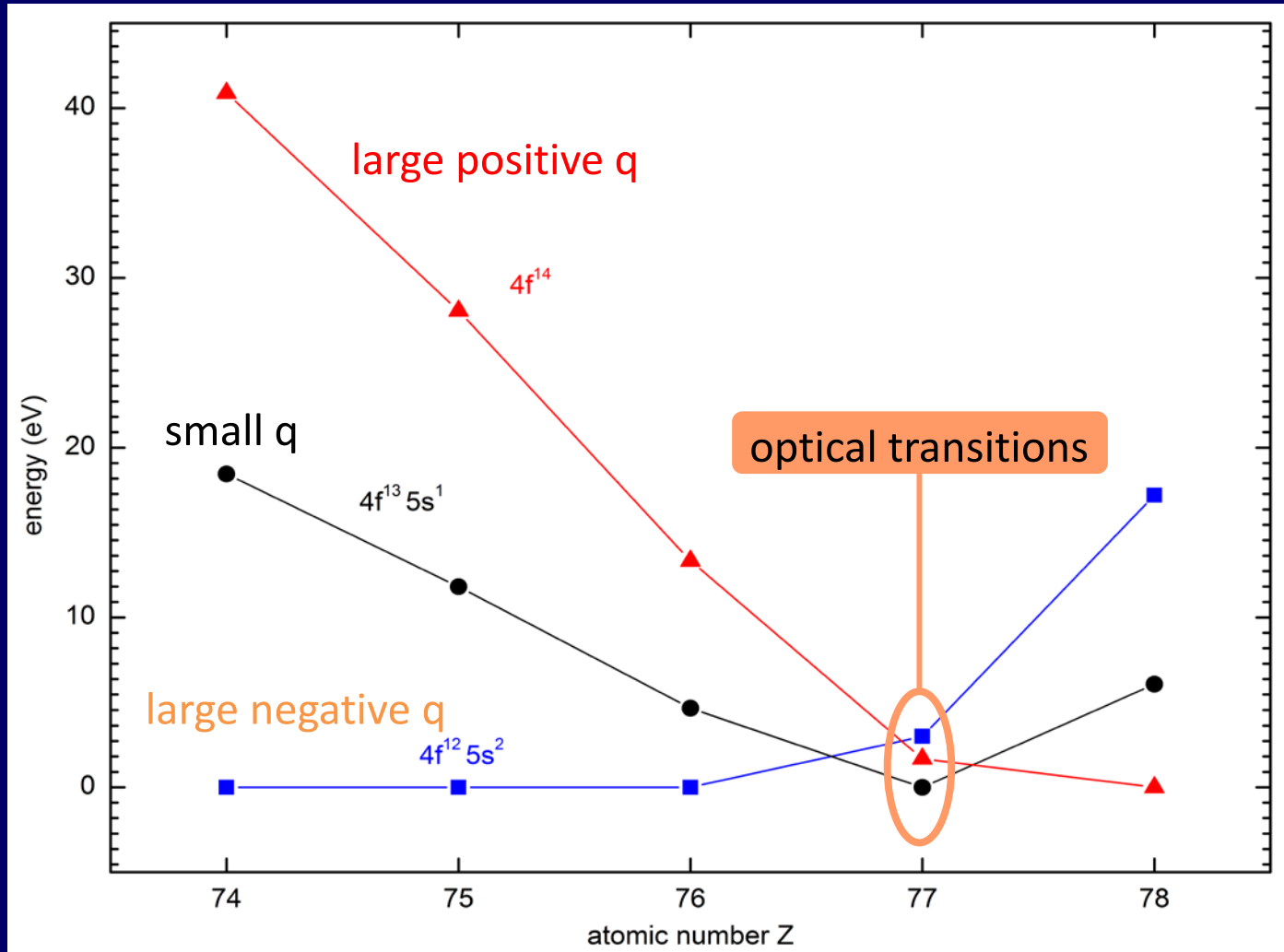


# Excitation yield vs. electron beam energy



## Metastable-aided electron-impact ionization (MAEII)

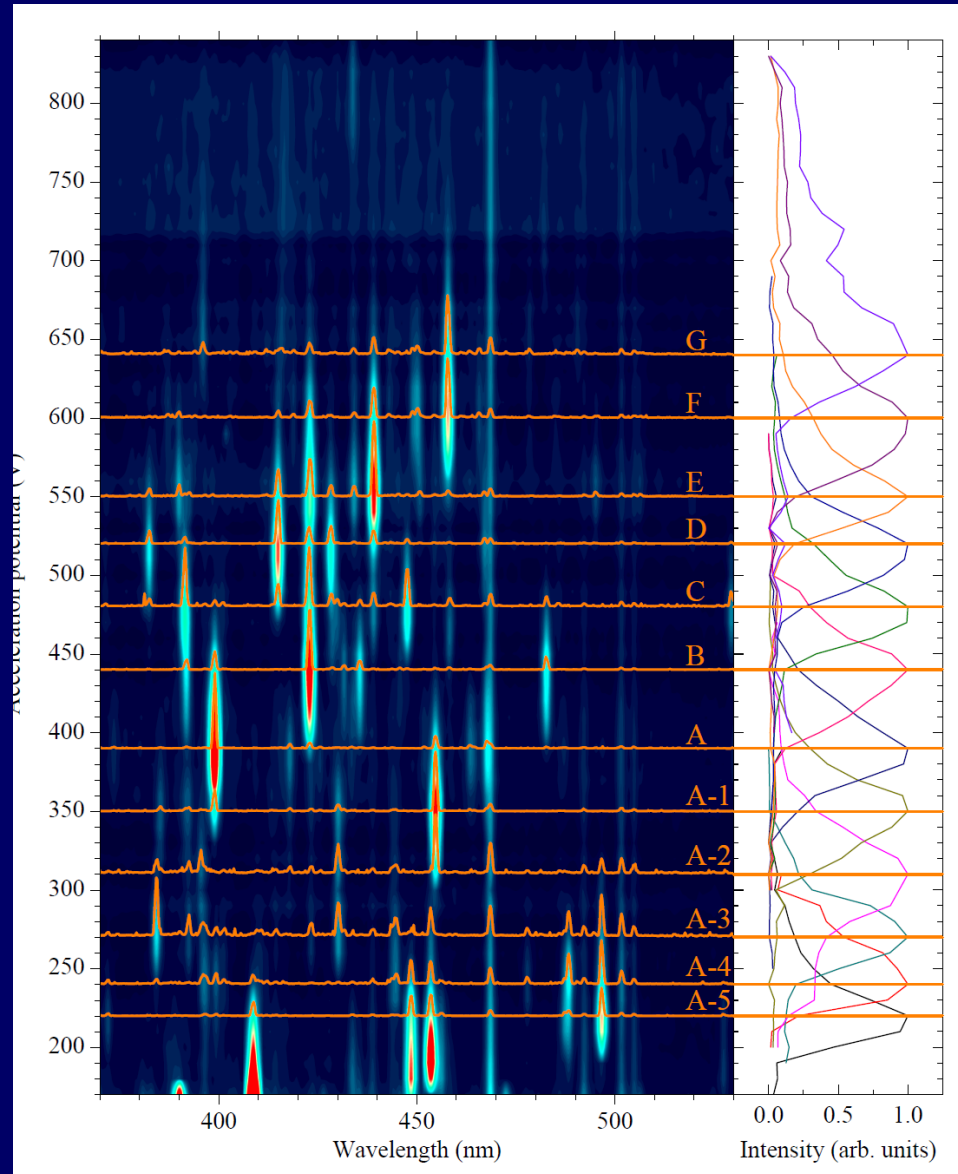
# Level crossings in $\text{Ir}^{17+}$ for $\alpha$ -clock



$\text{Ir}^{17+}$ :  $q \sim 740\,000\text{ cm}^{-1}$   $\longleftrightarrow$   $\text{Hg}^+$ :  $q \sim 52\,200\text{ cm}^{-1}$

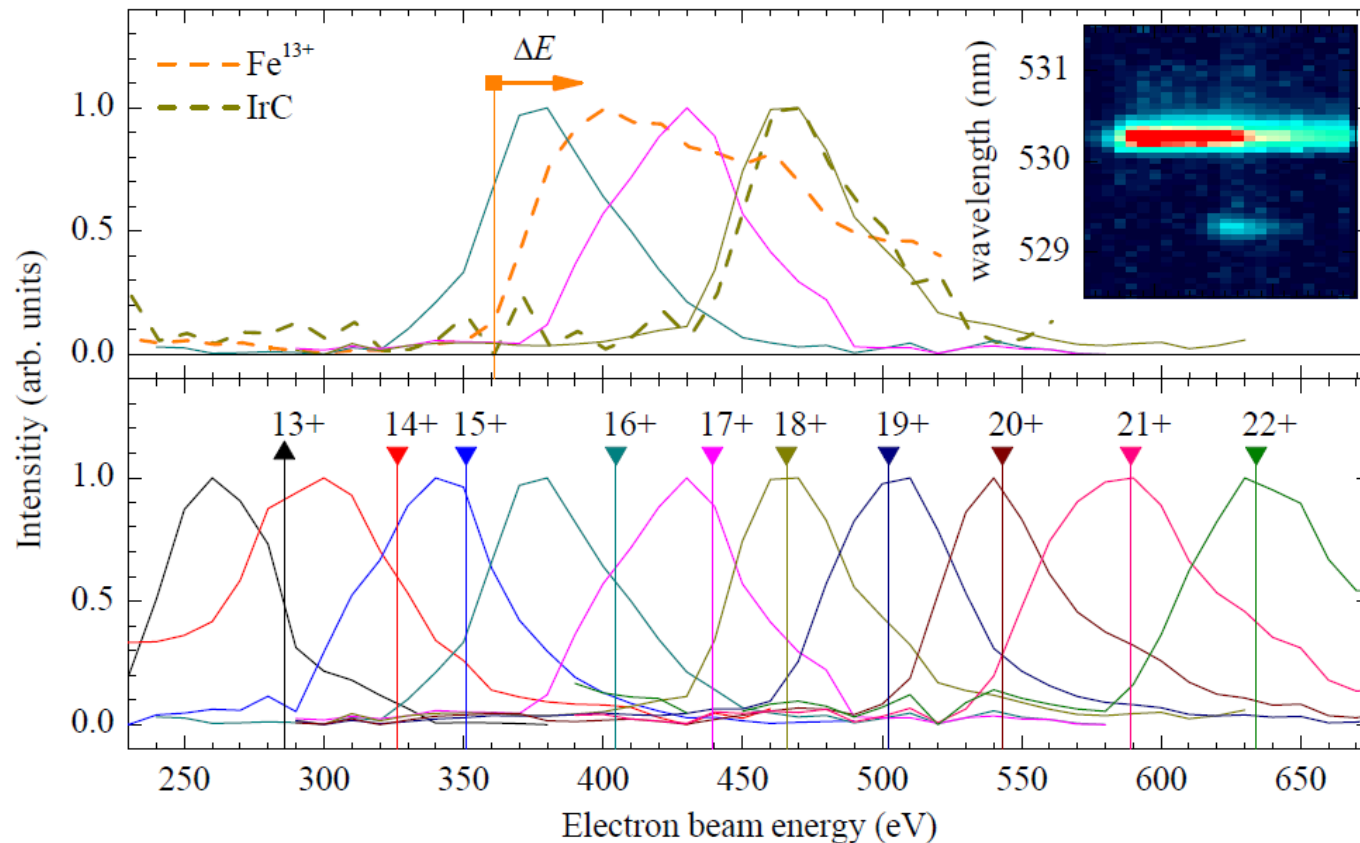
Predictions: J. C. Berengut *et al.*, PRL **106**, 210802 (2011)

# Level crossings at $\text{Ir}^{17+}$ provide $\alpha$ sensitivity



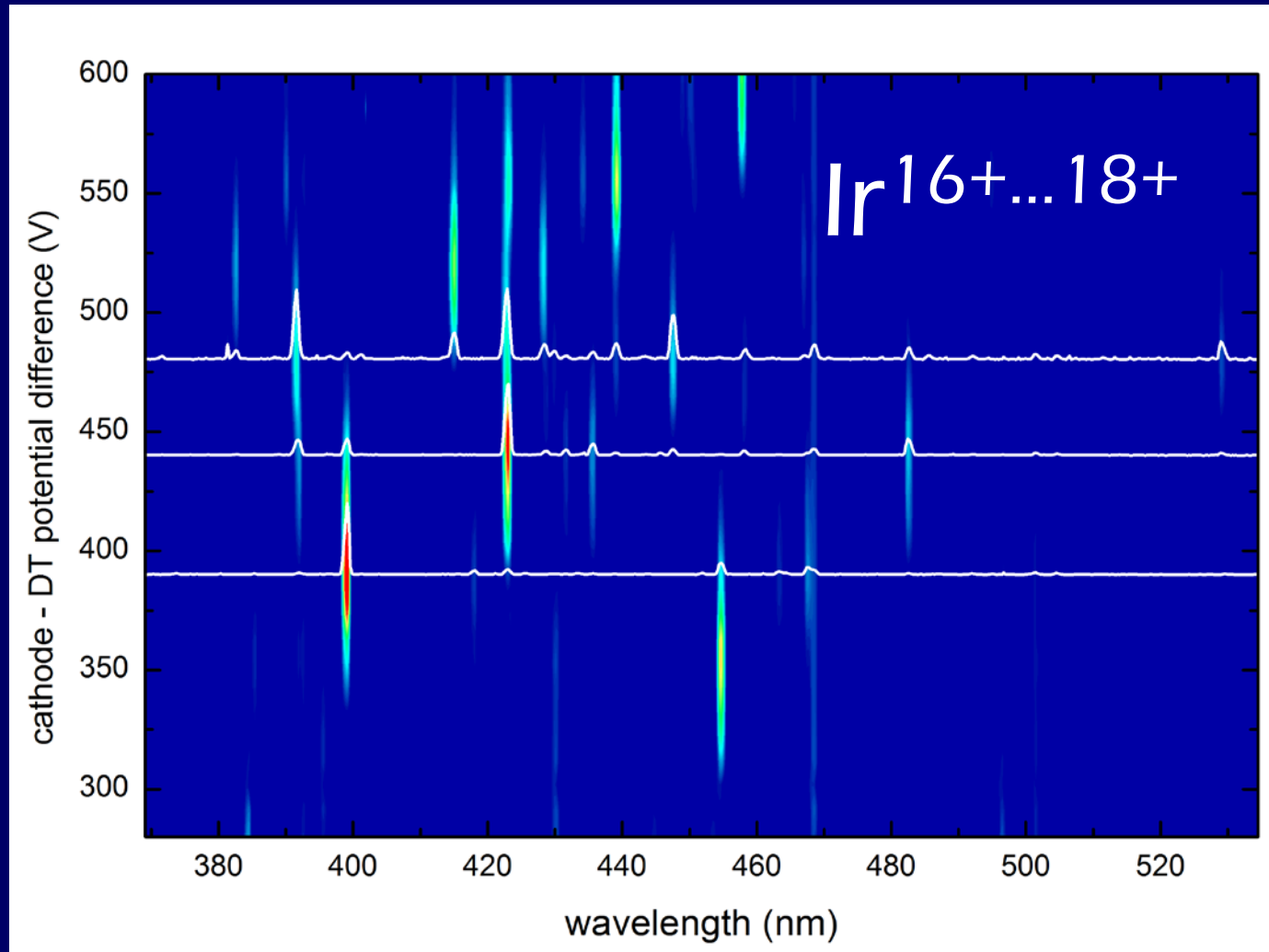
- With increasing charge state, reordering of levels takes place
- 4f levels go below 5s at  $Z \approx 77$  (Berengut *PRL* 2011)
- Levels of opposite parity cross:  $4f^{12} 5s^2$ ,  $4f^{13} 5s$ ,  $4f^{14}$
- M1, E1, E2, M2, M3 transitions become possible

# Searching for the right charge state



- By changing the electron beam energy, new charge states stepwise appear
- Uncertainties in both experimental threshold energy and theoretical predictions of ionization potentials

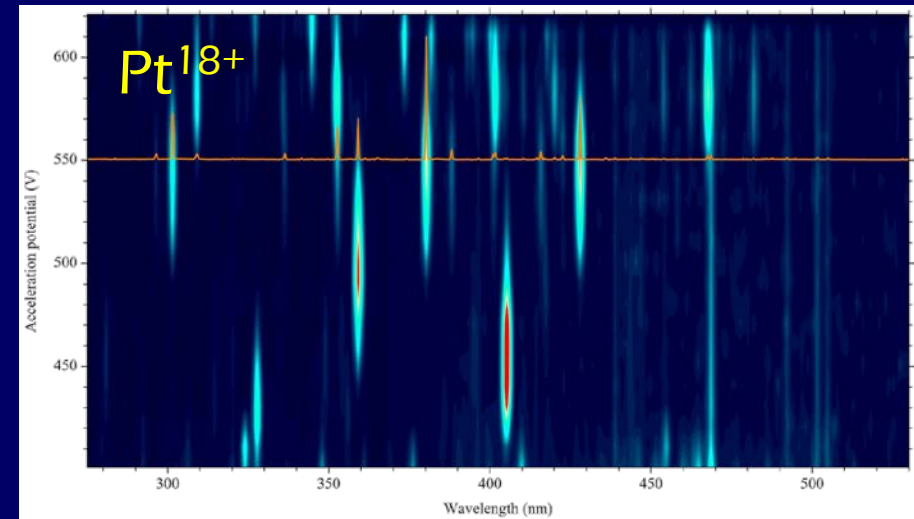
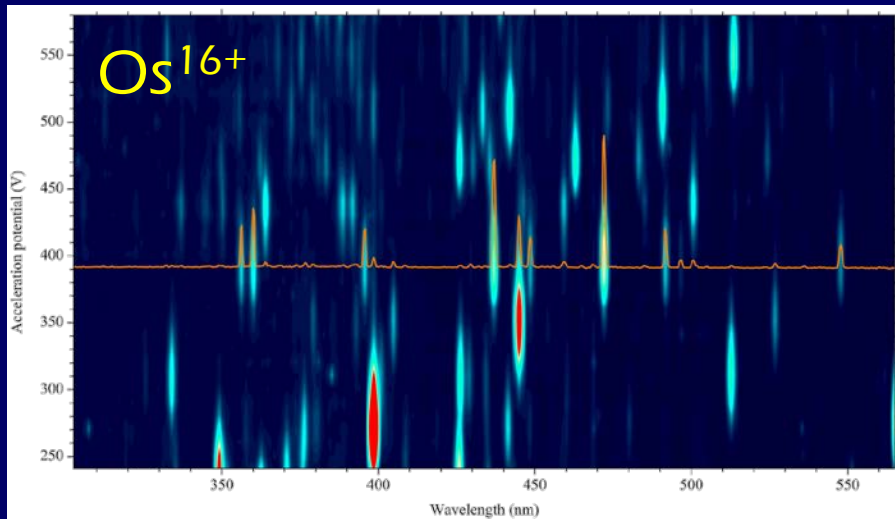
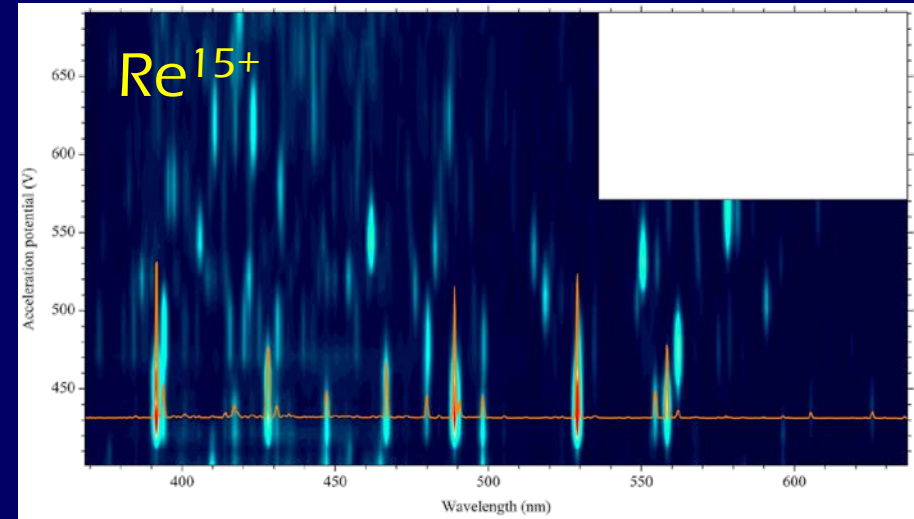
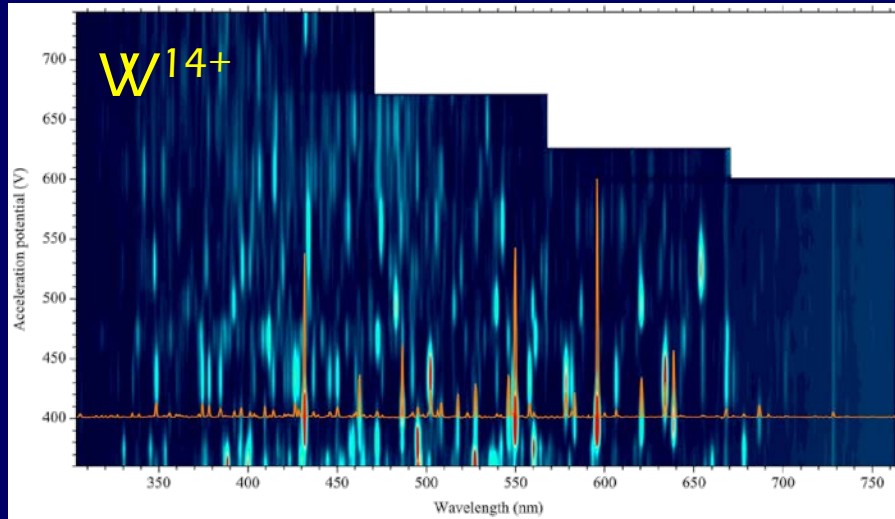
# Visible spectra of M1 lines in Ir ions



- First ever observations of such ions
- Line identification based on theory is unreliable



# Optical spectral maps Nd-like ions



Isoelectronic sequence studied in detail to find analogies

# Line identification through M1-scaling functions on Nd-like isoelectronic sequences

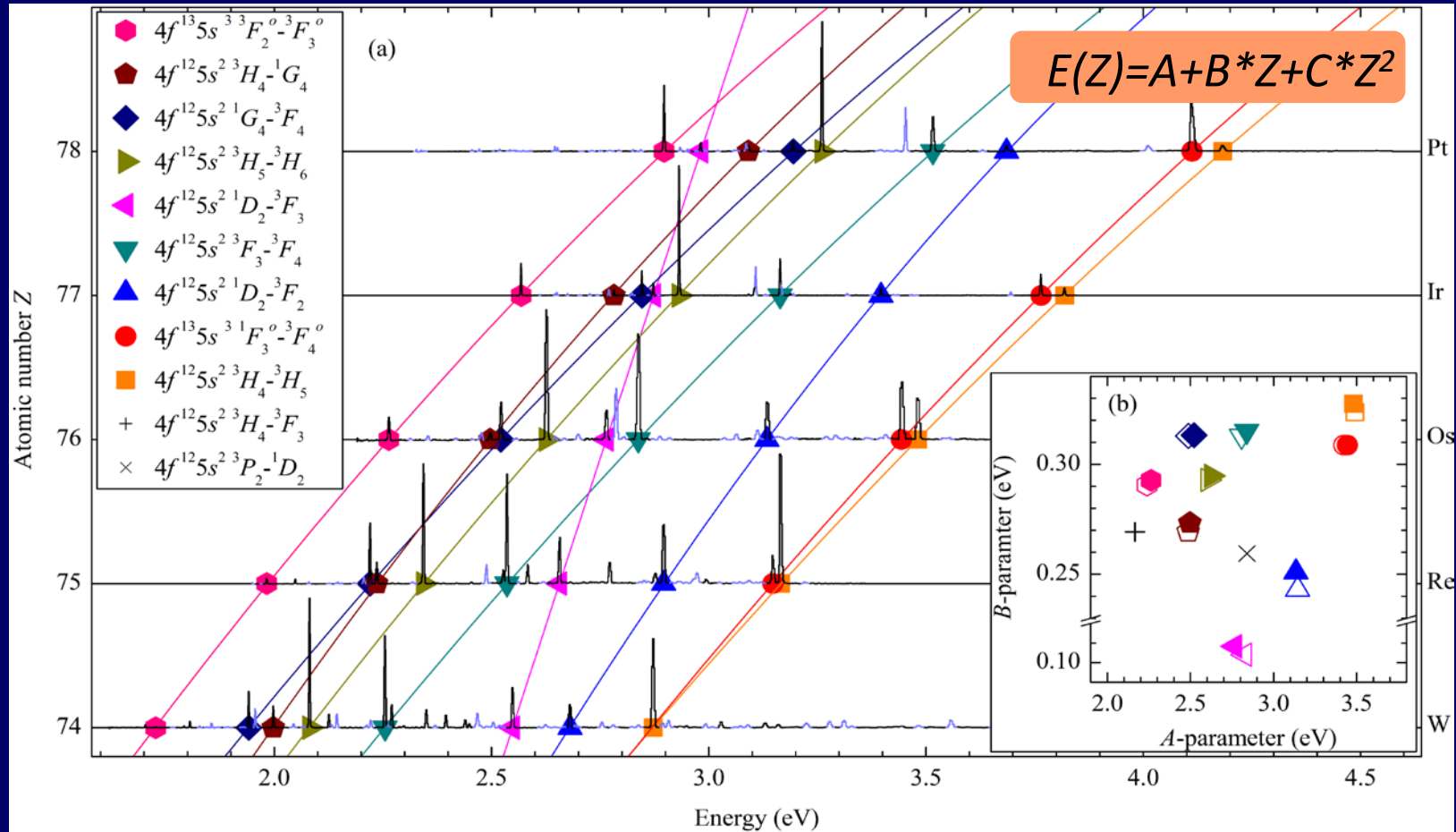
Pt

Ir

Os

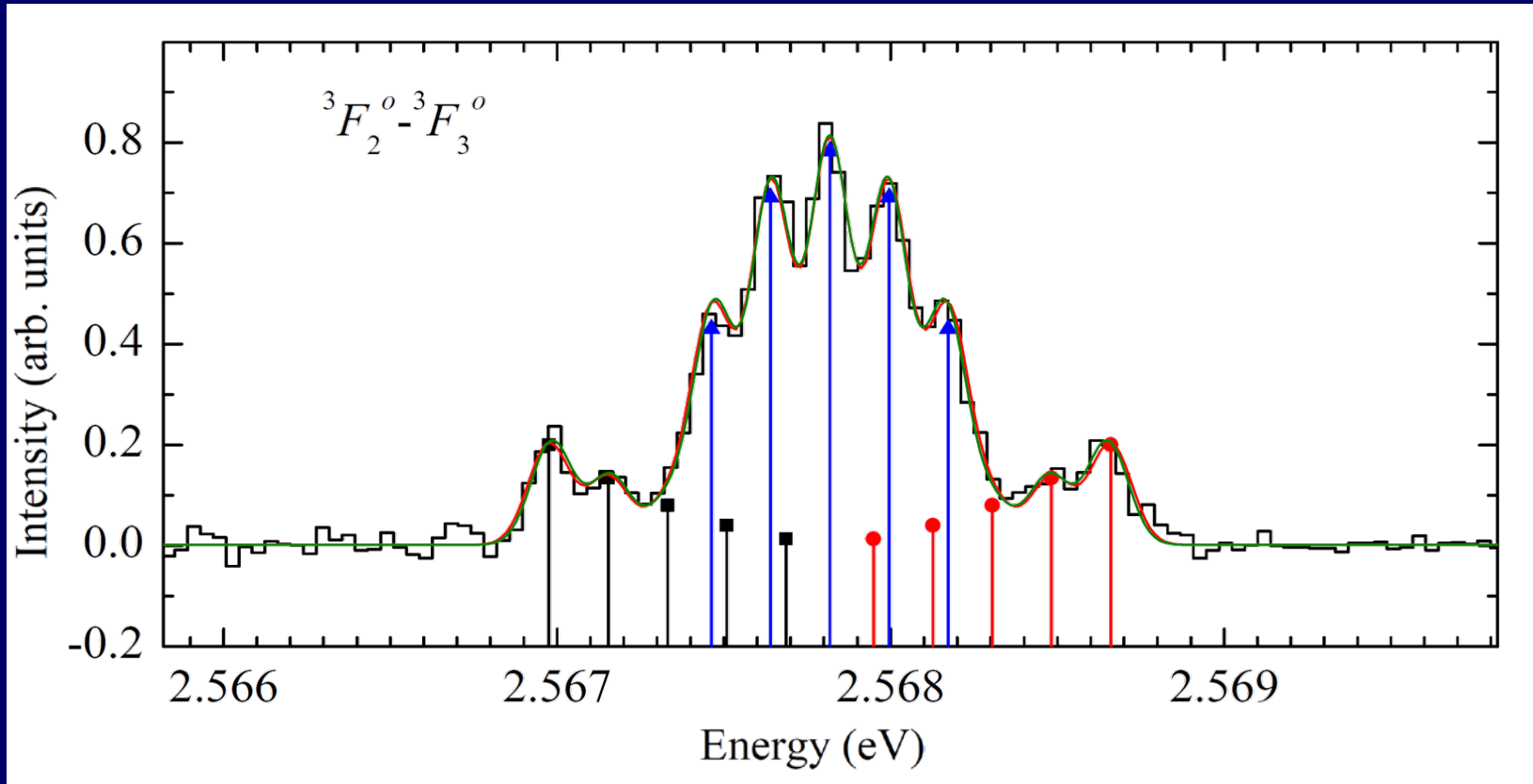
Re

W



Comparison between theoretical and experimental scalings  
allow us to identify the transitions and fill the Grotrian diagram

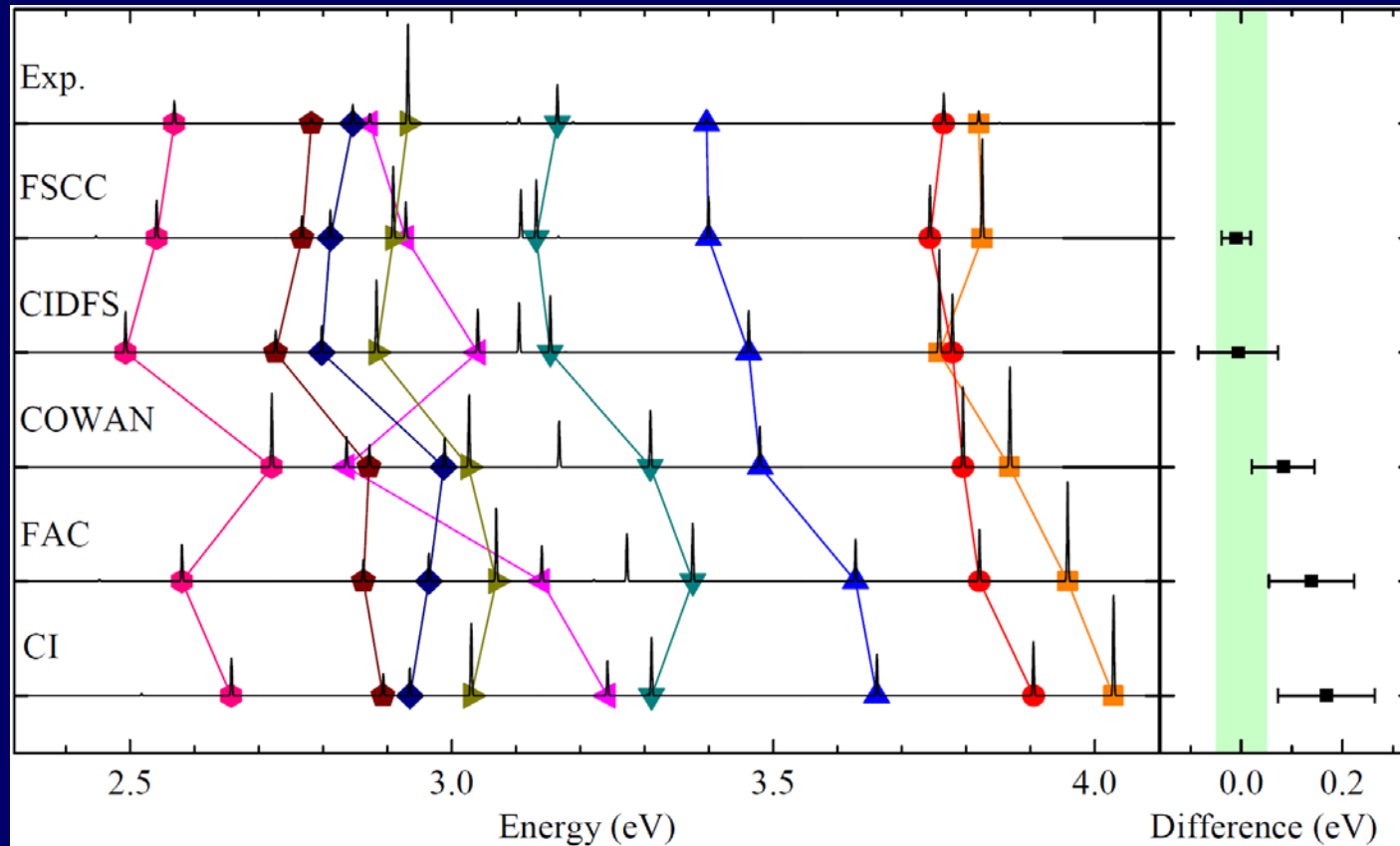
# Line identification through $g$ -factor fits



Magnetic field causes large Zeeman splitting providing an additional criterion for identification of the lines

$$\sum_{\Delta m=-1,0,1} A_{\Delta m} \sum_{-J \leq m_J \leq J} \langle J \ m_J \ 1 \ \Delta m | J' \ m_J + \Delta m \rangle^2 \times \exp \left( - \frac{(E - E_0 - \mu_B B (m_J (g - g') + \Delta m g'))^2}{2w^2} \right)$$

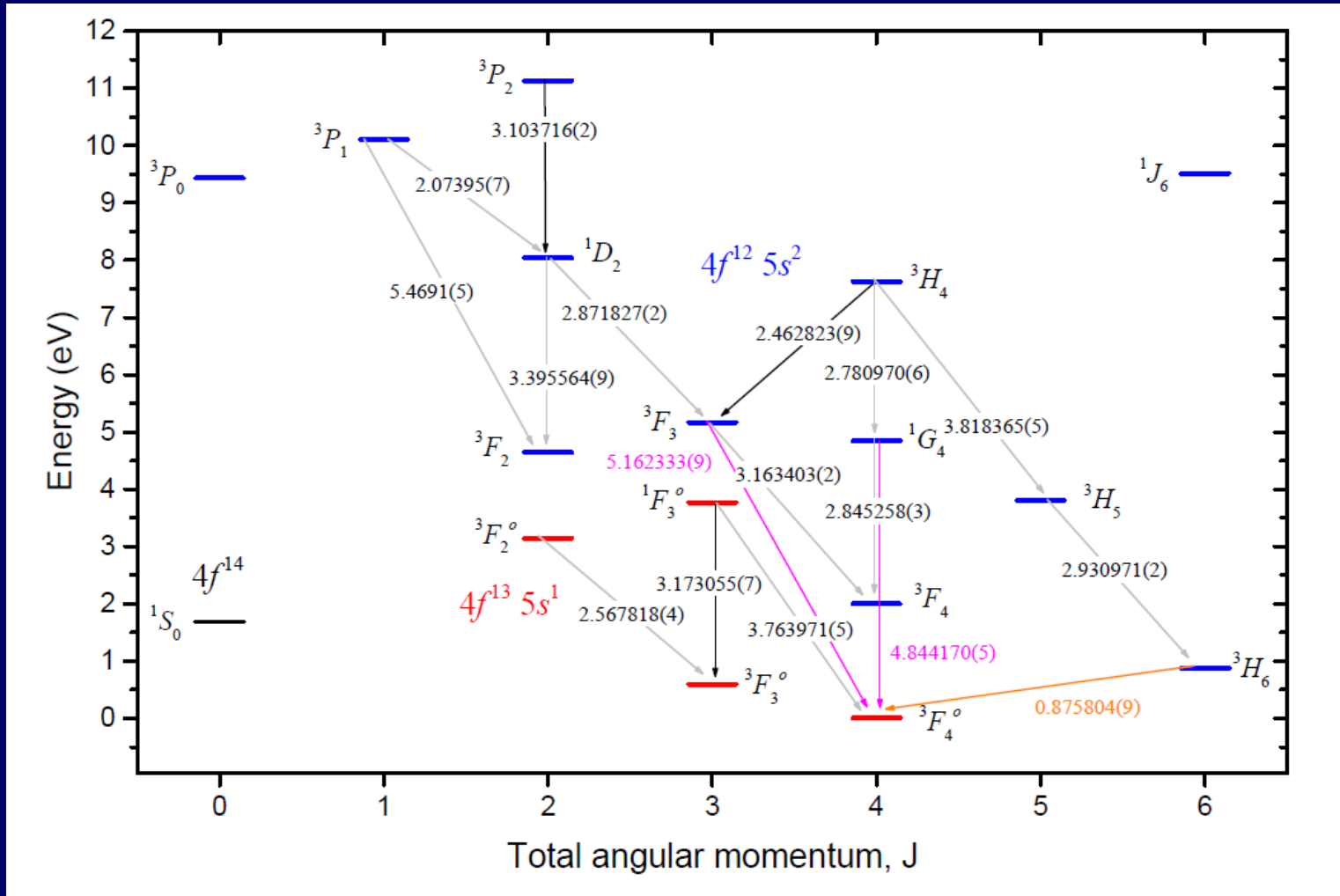
# Comparison between theories



- Fock-space coupled cluster calculation (A. Borschevski) shows agreement with experimental result at a level suitable for identification.
- Its deviations from experiment are smaller than the average separation between spectral lines (as given by the green band).

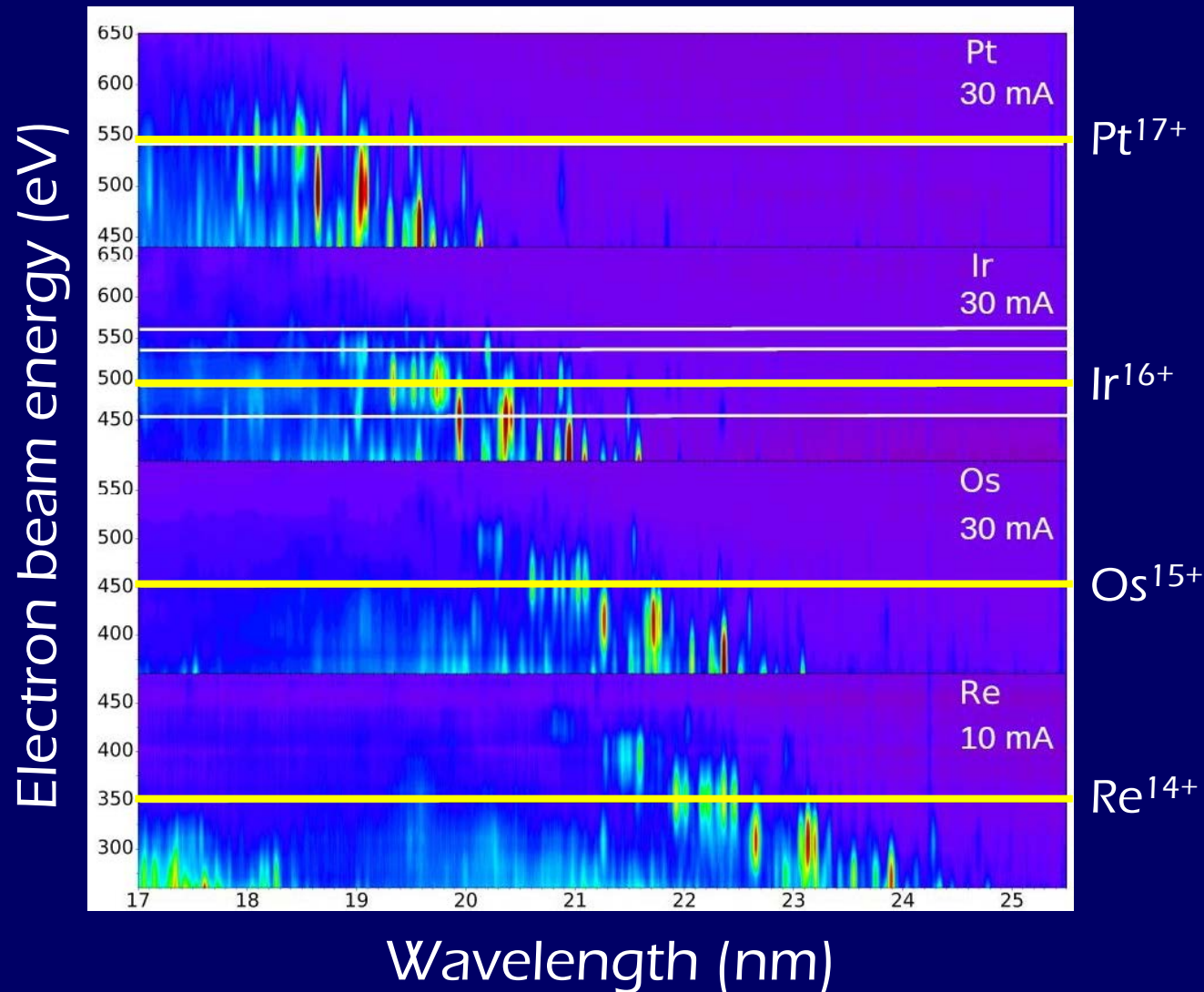


# New data on $4f^{14}$ , $4f^{13}5s$ and $4f^{12}5s^2$ for $\text{Ir}^{17+}$



Arrows: Black, identified M1 lines; magenta, tentatively identified E1; orange, inferred M2/E3 clock transition; gray, previously identified. Unconnected fine-structure levels taken from FSCC calculations.

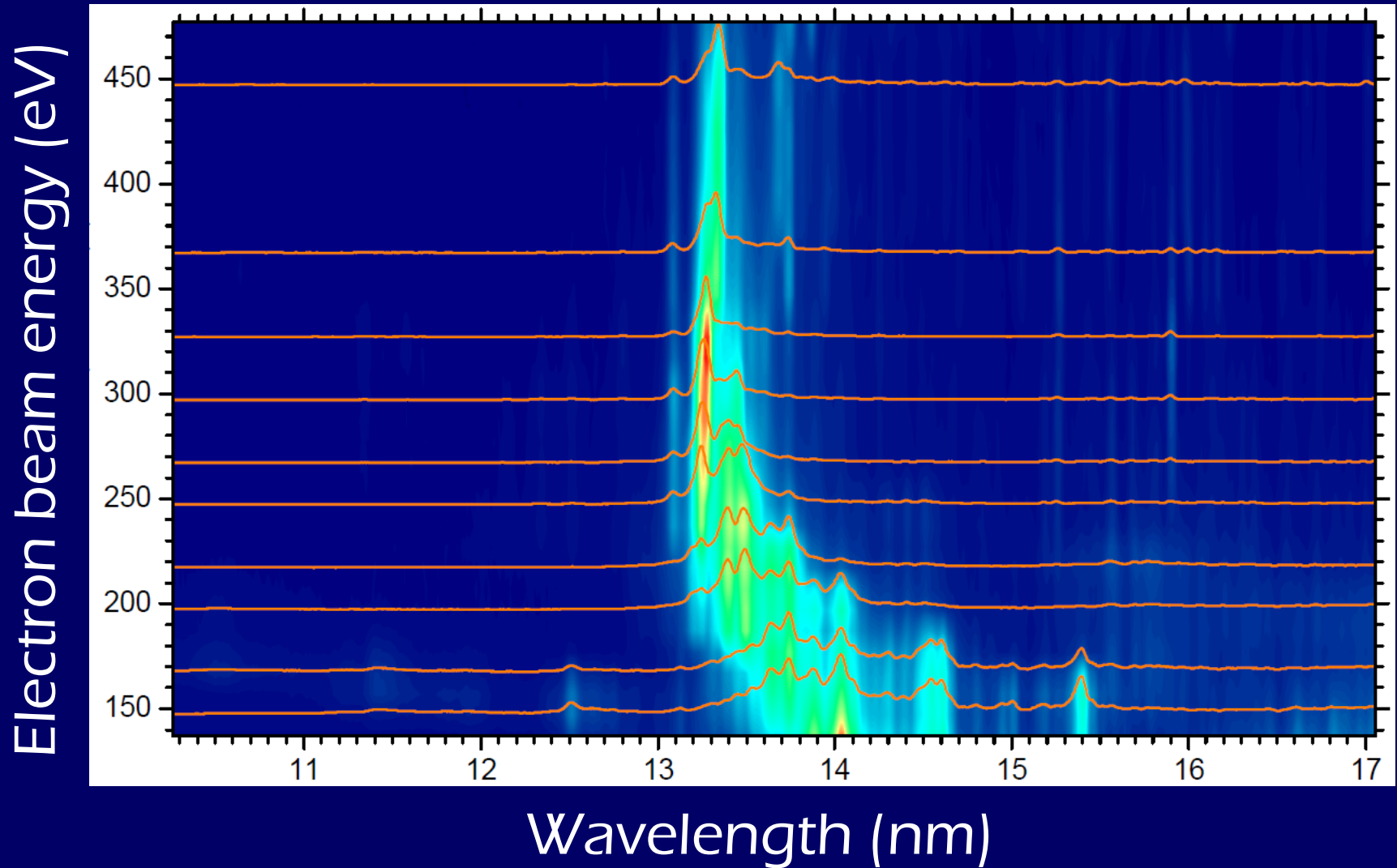
# Pm-like (61 electrons) isoelectronic sequence



Isoelectronic sequence studied in detail to find analogies

# Understanding optical and EUV spectra of tin ions

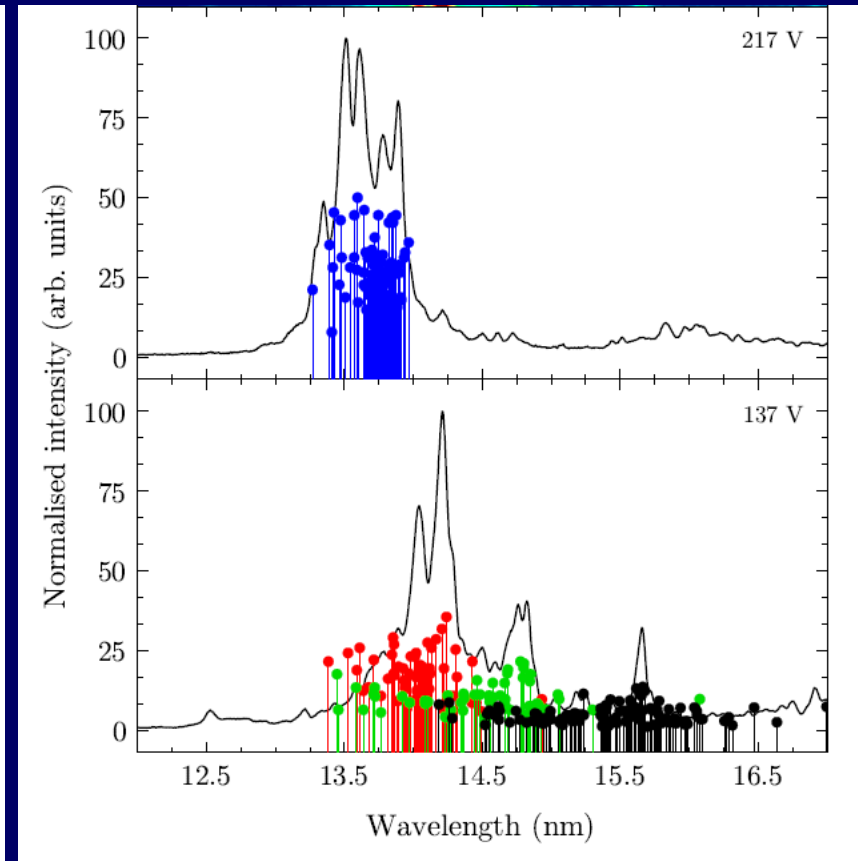
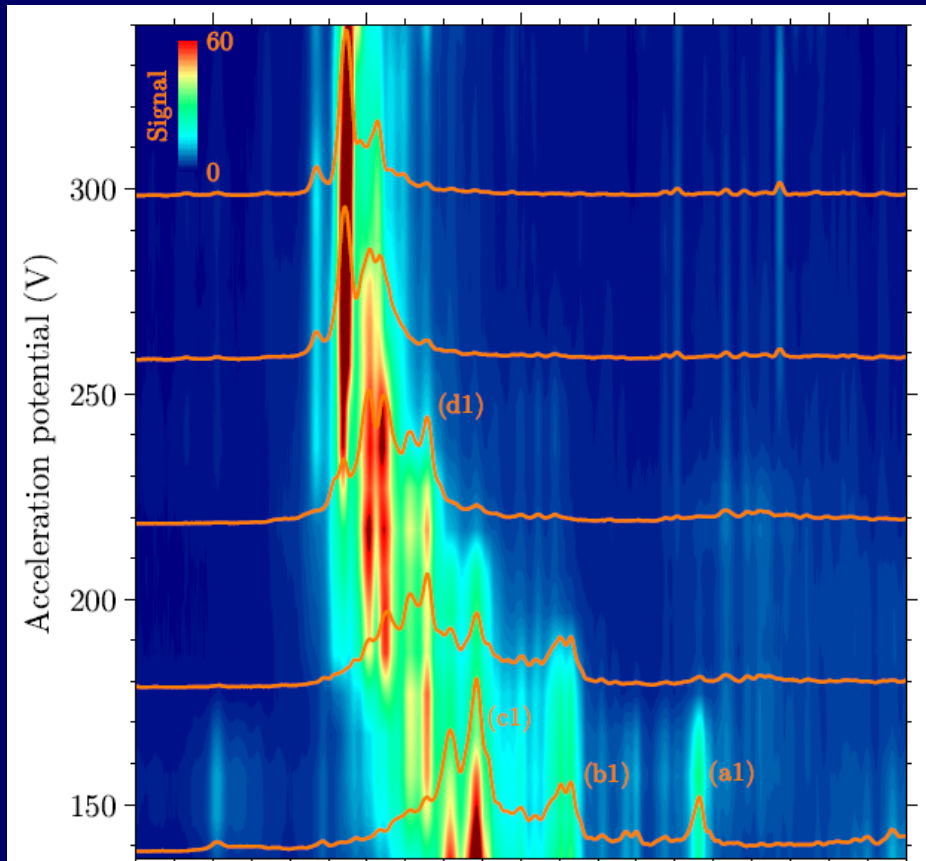
# Understanding Sn spectra



H. Bekker et al., J. Phys. B **48**, 144018 (2015)

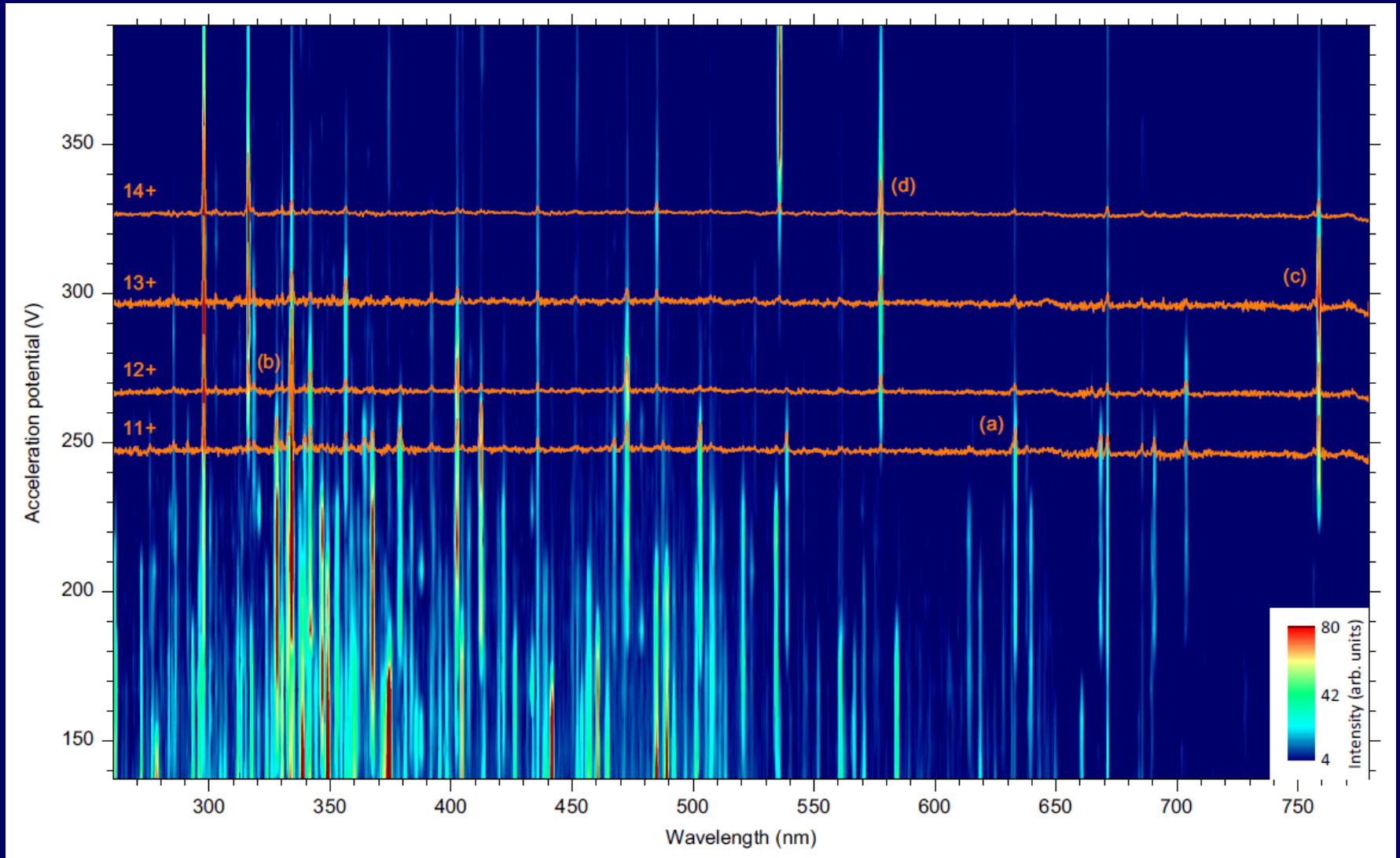


# Understanding Sn spectra



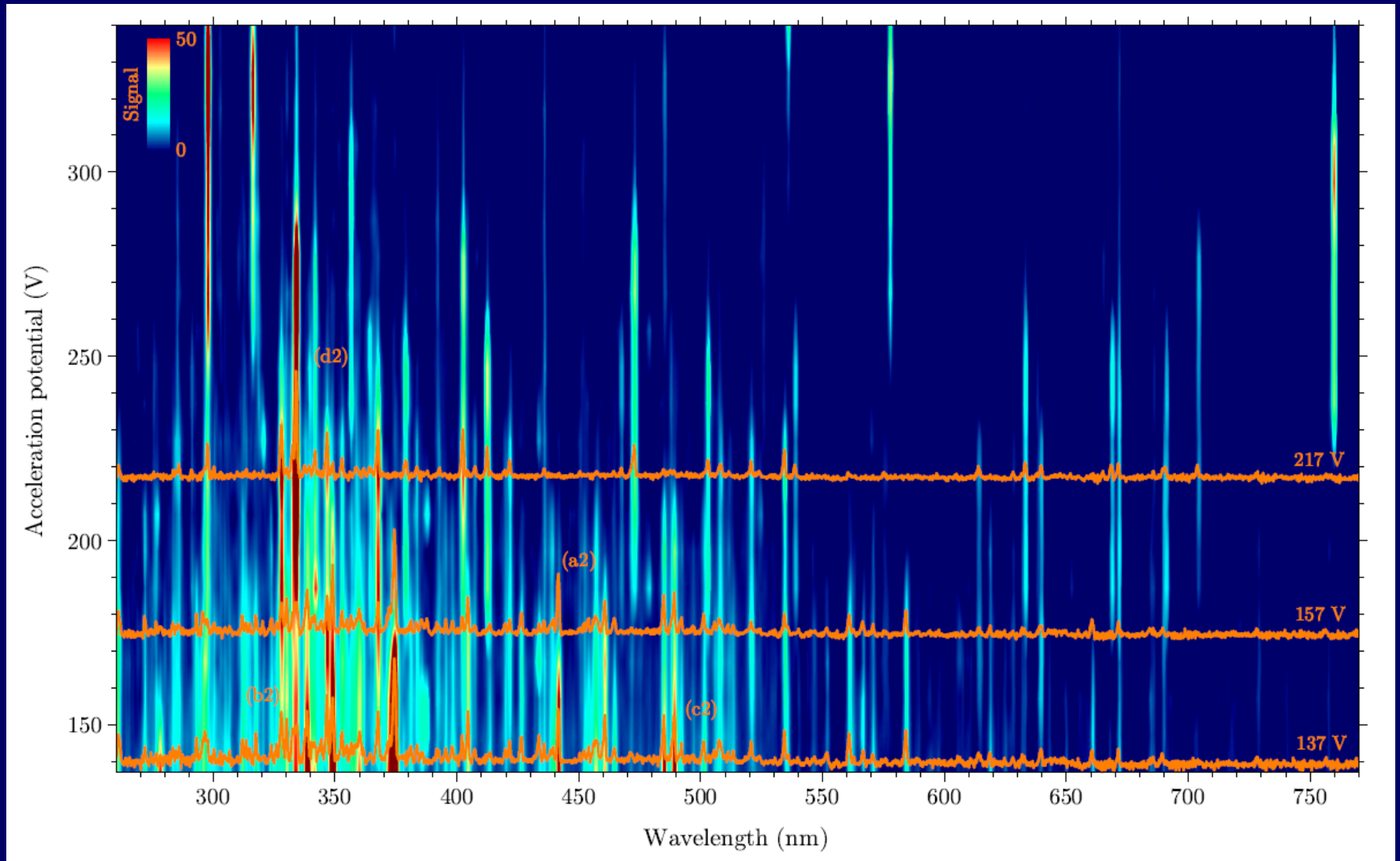
F. Torretti, ARCNL, in preparation (2016)

# Understanding Sn spectra



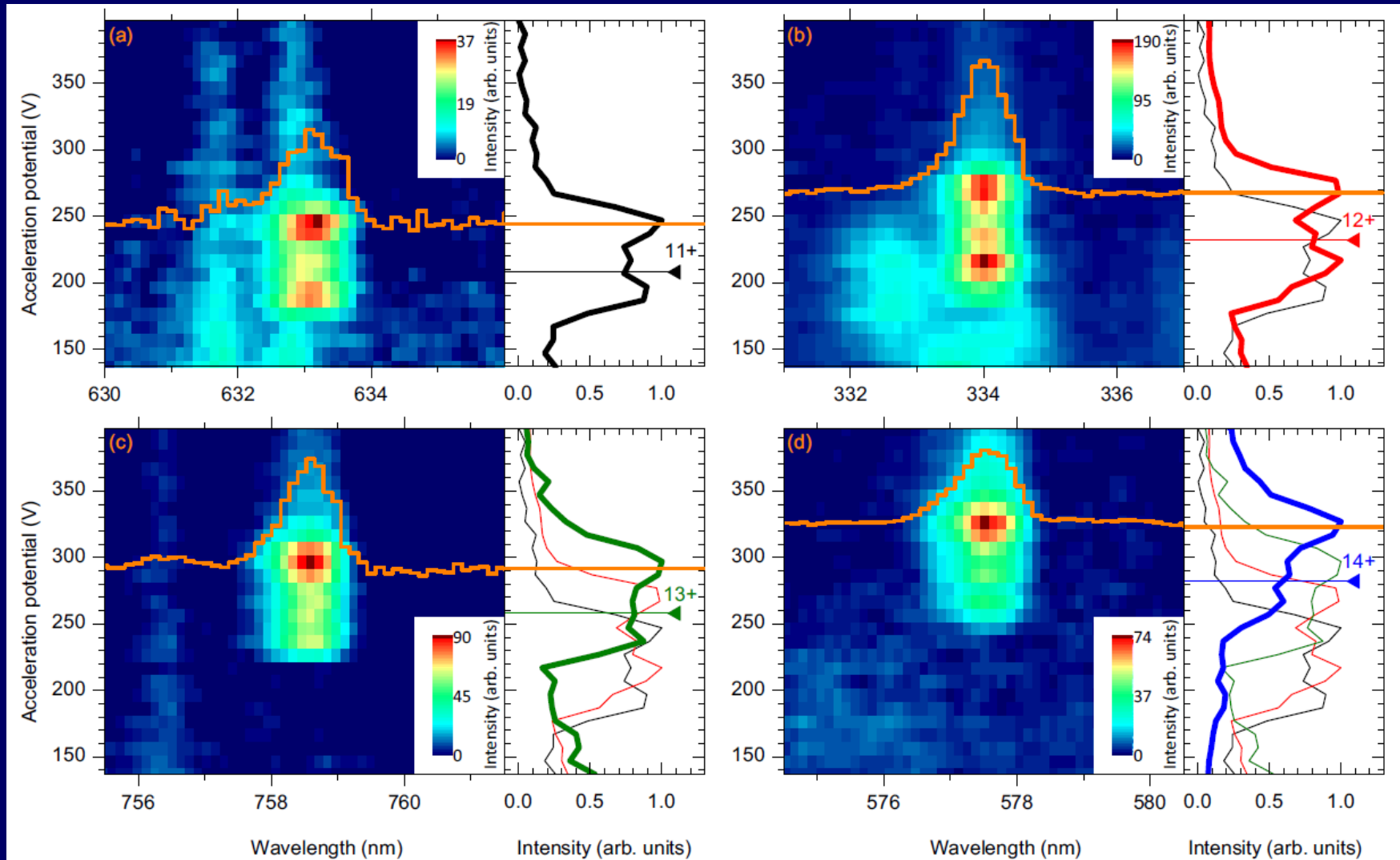
A. Windberger et al., Phys. Rev A **94**, 012506 (2016)

# Understanding Sn spectra



F. Torretti, ARCNL, in preparation (2016)

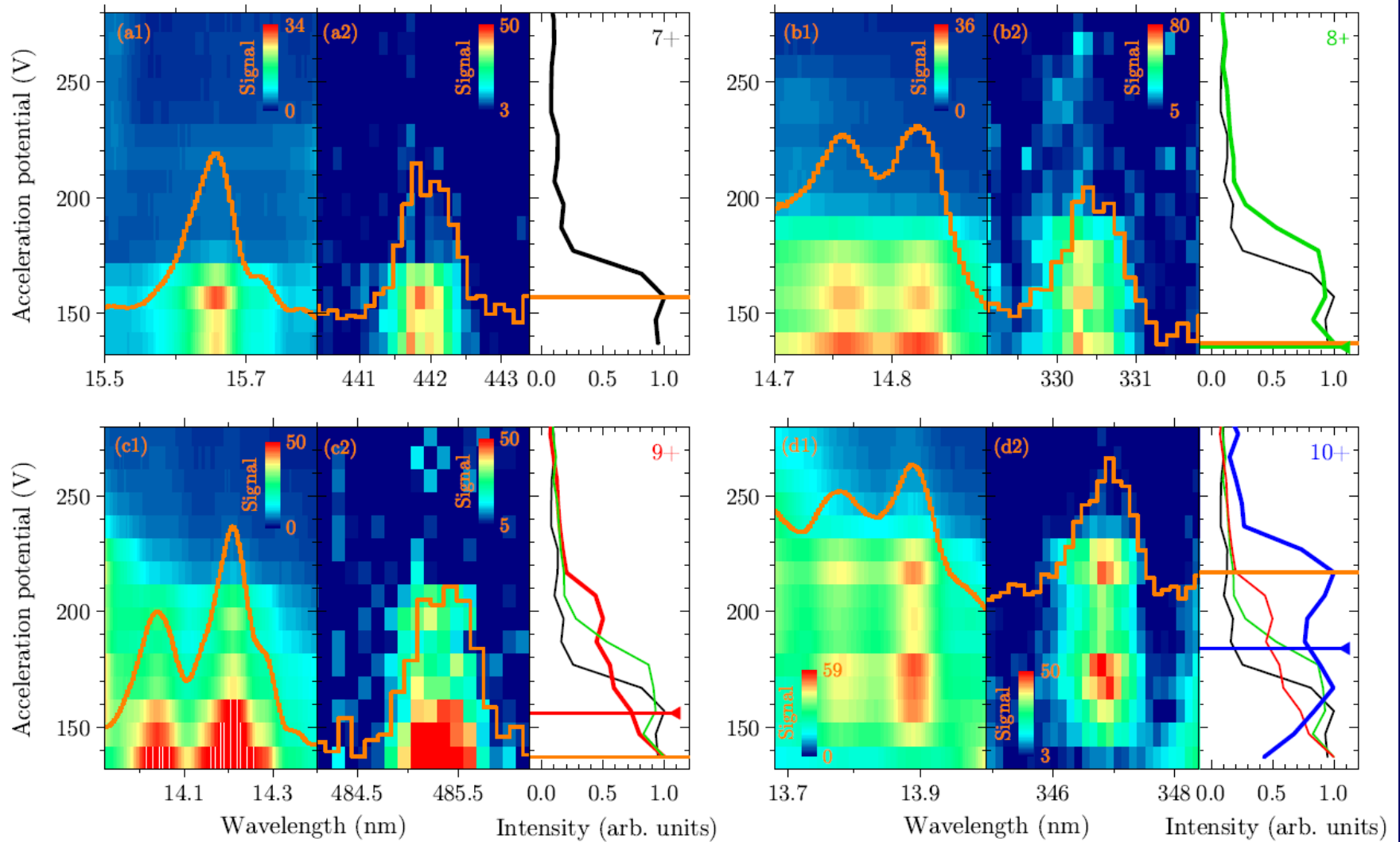
# Understanding Sn spectra



A. Windberger et al., Phys. Rev A **94**, 012506 (2016)

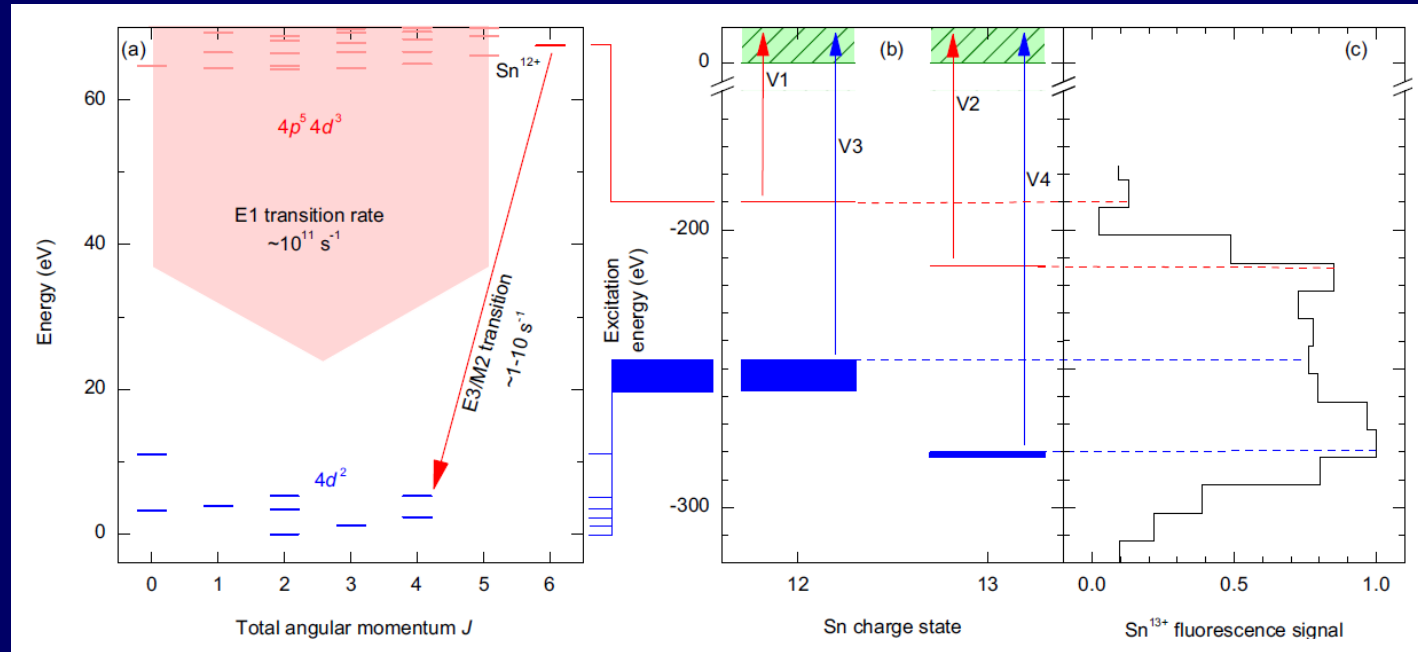


# Understanding Sn spectra



F. Torretti, ARCNL, in preparation (2016)

# Sn spectra: role of metastables



- Metastable states modify ionization dynamics and have a strong leverage in level populations and charge state
- Branching ratios and level couplings strongly depend on detailed level spacing
- Collisional-radiative modeling requires accurate atomic physics data

A. Windberger et al., Phys. Rev A **94**, 012506 (2016)

# Conclusions from VIS-EUV spectroscopy

- Careful analysis of **charge-state resolved optical and EUV spectra** challenges some earlier **identifications** based on transient plasmas
- **Fock-space coupled cluster (FSCC) and improved configuration interaction calculations (CI)** show acceptable ab-initio accuracy, **easing identification**
- By **calibrating Cowan-code parameters** on the basis of experimental optical and EUV spectra **semi-empirical line identifications** can be completed

# Summary

- Role of many-electron correlations is only qualitatively understood , but quantitative ab-initio calculations are challenging and require novel approaches (FSCC, improved CI and RMBPT)
- Open p, d ,f subshells challenge theory and experiment due to multi-electron resonant free-bound interactions
- Photorecombination, photoionization, electron-impact excitation as well as ionization, and charge exchange are needed to model the data
- Charge-state and electronic state-resolving studies are needed to guide theory

# Thanks to:

## MPIK

H. Bekker, A. Windberger, O. Versolato,  
S. Bernitt, R. Steinbrügge, J. Rudolph,  
C. Beilmann, S. W. Epp, M. C. Simon,  
C. Shah, T. M. Baumann, K. Kubicek,  
V. Mäckel, P. Mokler, J. Ullrich, T. Pfeifer,  
JRCLU

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